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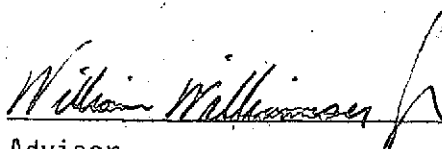
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Calculation of Total Electron Excitation Cross-Sections and
Partial Electron Ionization Cross-Sections for the Elements

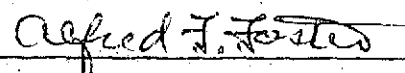
by

T. J. Greene

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Advisor



Dean of the Graduate School

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ABSTRACT

Computer programs are used to calculate the total electron excitation cross-section for atoms and the partial ionization cross-section. The calculation is done in the following manner. Each of the approximations listed below results in an expression for a scattering amplitude, involving the atomic wave function of the target. These amplitudes are simply related to the differential cross-sections which are integrated to give the total excitation (or partial ionization) cross-section for the collision.

The approximations to the scattering amplitude used are

Non-Exchange Excitation:

- 1) Born
- 2) Bethe
- 3) Modified Bethe

Exchange Excitation

- 1) Ochkur

Non-Exchange Ionization

- 1) Coulomb - Born.

The atomic wave functions used are Hartree-Fock-Slater, (HFS) functions for bound states and the coulomb wave function for the continuum.

The programs are presented and some results are examined.

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I. INTRODUCTION

1. History and Significance of the Problem.

The purpose of this research is to calculate the total electron excitation cross-section and the partial ionization cross-section for atoms. Symbolically the excitation process is written:

$$Z(n_i \ell_i m_i) + e \rightarrow Z(n_f \ell_f m_f) + e \quad (1)$$

The problems of computing excitation and ionization cross-sections have been of interest for some time. An attempt to compute cross-sections for excitations to the continuum (i.e. ionization) was made by Thomson in (1912). His classical theory of ionization of atoms has been recently restudied by Rudge (1968) as a result of a renewal of interest in semiclassical calculations as approximations to more elaborate quantum mechanical calculations.

Some of the early papers in Quantum Mechanics were also concerned with the problem of atomic excitation calculations. The papers of Born in (1926) and Oppenheimer in (1928) are particularly noteworthy.

As the field of astrophysics has advanced in sophistication interest in atomic cross-section calculations has further increased. Bates mentioned in (1950) that quantitative information on the cross-section associated with excitation and ionization by electrons is necessary in connection with several astrophysical problems. In particular such information is necessary for an understanding of the observed spectral characteristics of aurorae and in connection with investigations of the solar corona and gaseous nebulae. The subject

of gaseous nebulae is discussed by Cyszak (1968) who mentions that accurate transition probabilities and collisional cross-sections are necessary for proper interpretation of the properties of nebulae.

These are some of the needs for excitation cross-sections. There are two methods of determining such cross-sections; experimental measurements or theoretical calculations.

Certain inelastic collisions of electrons with atoms have been studied experimentally and some cross-section information has been obtained (Kieffer (1967)), but experimental measurements, particularly of the absolute values of the excitation cross-sections, are in general very difficult. Furthermore, exceptional difficulties are encountered in the experimental measurements in many cases of particular interest (Heddle (1968)).

Three main categories of experimental methods have been used (see Moiseiwitsch and Smith (1968)). In the first method intensities of spectral lines excited by an electron beam are measured. The measurements in this case effectively determine an optical excitation function as opposed to the desired electron excitation cross-section. The fundamental differences between these two quantities arise due to the effects in the photon measurements of cascades from higher levels with several channels for decay, which produce an anisotropic radiation pattern. A principal problem in these measurements is absolute calibration of the optical system.

A second method is based on the deactivation of "metastable" states at a metal target. The electrons ejected from the metal target provide information. The difficulties of this method are connected with determining the efficiency of collection and conversion of metastable atoms at

the metal target.

The third experimental method involves a study of the energy loss spectrum of scattered electrons. Here an electron beam of definite energy is passed through a gas and the energy spectrum of electrons scattered at a particular angle with respect to the beam axis is measured by use of an electron energy analyzer. The principal difficulties here arise from the necessity of taking data at many angles as well as over a range of energies.

As is pointed out by Bely (1970), reviews of experimental methods have been written by Fite (1962), Moiseiwitsch and Smith (1968), and Heddle and Kessing (1968).

The difficulties encountered in a theoretical approach are immediately obvious in view of the fact that an electron target atom system is essentially a many-body system. The particular difficulties involved and the approximations made in an attempt to overcome these difficulties will be one of the concerns of the present research.

At the outset we are forced to recognize that the problem of electron impact excitation of atoms is so complex that, even for the case of electron collisions with atomic hydrogen, there is no exact solution known for the excitation cross-section of the two lowest states. Therefore, to assess the accuracy of various approximate calculations the only method available is that of comparing the cross-sections obtained in the various calculations with one another and with the limited experimental data available.

The data that is available, both experimental and theoretical, has recently been collected by the Information Center of the Joint Institute

of Laboratory Astrophysics (JILA), and the Oak Ridge Atomic and Molecular Information Center. A series of reports published by JILA emphasize that for many elements and transitions there is in fact no data available (see Kieffer (1967)).

This fact is again emphasized in a recent article by Athay (1972). The author states, "We have no information either experimental or theoretical of collision cross-sections for (these) forbidden transitions."

Motivated by the need (expressed in particular by astrophysicists) but restricted by the complexity of the problem, the present research obtains inexact but reasonable excitation cross-section values for all elements by use of various approximations.

II. WAVE FUNCTIONS

A fundamental difficulty in any problem involving atoms is that of obtaining accurate atomic wave functions. These are the solutions to the problem:

$$H\phi_A = E_A\phi_A \quad (2)$$

where H is the Hamiltonian operator incorporating all of the interactions of the constituents of the atom and the ϕ_A are the eigensolutions of this operator for the eigenvalues E_A .

The exact treatment of this problem requires the use of the proper Dirac Hamiltonian (i.e. the inclusion of relativistic effects) but this problem is so complex that the following assumptions are commonly made:

- I. It is assumed that the Dirac Hamiltonian can be approximated by the Schrödinger Hamiltonian. (This allows the wave function to be represented by a single function rather than the matrix of four functions required by the Dirac equation.)
- II. It is assumed that the particles move independently. (This allows the total wave function for the system of particles to be written as a product of one particle wave functions).
- III. It is assumed the electrons move in a central field due to the nucleus and all other electrons. (This allows the one particle wave functions to be separated into radial and angular components).

The separation of the radial and angular parts of the wave functions allowed by assumption III gives two equations. The spherical harmonics are the solutions of the angular equation. Thus the problem is reduced to finding the radial wave functions which solve the remaining radial equation.

We would expect these assumptions would be less valid and therefore our wave functions less accurate where

- relativistic effects are significant (i.e. Large Z)
- electron - electron interactions are more significant (i.e. large occupation numbers for given orbitals).

These expectations are confirmed by the comparison of experimental and theoretical energy values given by Herman and Skillman (1963) in Chapter (3) of their work.

1. Bound State Wave Functions

A technique for finding the radial wave functions for bound state electrons was developed by Hartree. His treatment involves assuming a form for the central field, solving the radial equations for the one particle wave functions, finding the field due to these wave functions and then comparing the calculated field with the assumed field. Where the two fields agree, to within some previously specified tolerance, the problem is considered solved. Otherwise, where the two fields do not sufficiently agree, the calculation is begun again using the computed field as the assumed field and computing a new field. The procedure is repeated until the desired agreement is obtained.

The Schrödinger Hamiltonian for an n -electron atom is given in atomic units (see Appendix II) as:

$$H = -\frac{1}{2} \sum_{i=1}^n \nabla_i^2 - \sum_{i=1}^n \frac{Z}{r_i} + \sum_{ij} \frac{1}{r_{ij}} \quad (3)$$

The prime indicates that the summation is over all pairs, each pair being included once and the term $i=j$ being omitted.

In the Hartree model the total wave function for the system is assumed to be a product of single electron wave functions.

$$\Phi = \phi_a(\vec{r}_1) \cdots \phi_z(\vec{r}_n) \quad (4)$$

The third term in H represents the electron-electron interaction. The charge density of the j^{th} -electron is $|\phi(r_j)|^2$. We can then make the replacement

$$\sum_{ij} \frac{1}{r_{ij}} \rightarrow \sum_i \left\{ \sum_j \int dr_j \frac{|\phi(r_j)|^2}{r_{ij}} \equiv u(r_i) \right\} \quad (5)$$

The Schrödinger equation for this system is then

$$\sum_{i=1}^n \left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + u(r_i) \right) \prod_k \phi_{a_k}(\vec{r}_k) = E \prod_k \phi_{a_k}(\vec{r}_k) \quad (6)$$

This equation separates into the set of n -equations

$$\left[-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + u(r_i) \right] \phi_{a_i}(\vec{r}_i) = E_i \phi_{a_i}(\vec{r}_i) \quad (7)$$

(A rigorous derivation of this approximation using a variational principle is given by Slater (1957)).

Let us notice that as assumed in Eq. (5) the spherical harmonics solve the angular equation and the problem remaining is the radial equation:

$$\left[\frac{d^2}{dr^2} + 2 \left(E_{nl} + \frac{Z}{r} - u(r) \right) - \frac{l(l+1)}{r^2} \right] P(Nl;r) = 0 \quad (8)$$

For computational ease in the numerical procedures required by the

Hartree model, this equation is traditionally written:

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} [Y(r) + Y_0(n\ell:n\ell:r)] - \epsilon_{n\ell,n\ell} - \frac{\ell(\ell+1)}{r^2} \right\} P(n\ell:r) = 0 \quad (9)$$

where

$$Y(r) = Z - \sum_{n'\ell'} q(n'\ell') Y_0(n'\ell':n'\ell':r) \quad (10)$$

and where $q(n\ell)$ represents the number of electrons in each shell.

$Y_0(n'\ell':n'\ell':r)$ is a spherically symmetric charge distribution of radial charge density $|P(n'\ell':r)|^2$. Eq. (9) is the Hartree self consistent field equation without exchange (H-EQ).

The Hartree equation may also be derived from the variational principle. For the present purpose the principle is expressed by the statement that if Ψ is an approximate wave function for the ground state of a system described by the Hamiltonian H , the closer Ψ approaches the true eigenfunction of the Hamiltonian the lower the approximate eigenenergy becomes; i.e.

$$E \leq \int \Psi^\dagger H \Psi \, d\tau / \int \Psi^\dagger \Psi \, d\tau \quad (11)$$

(For a more detailed statement of the principle see Landau (1958), Hartree (1957) or Gottfried (1966)).

The derivation is then the result of assuming the approximate wave function form $\Psi = \psi_a(\vec{r}_1) \cdots \psi_z(\vec{r}_n)$ and finding the best solutions of the Schrodinger equation by minimizing $\int \Psi^\dagger H \Psi \, d\tau / \int \Psi^\dagger \Psi \, d\tau$ subject to the condition $\int d\vec{r} |\psi(\vec{r})|^2 = 1$. This procedure again results in the Hartree equation and assures us that the Hartree eigenfunctions are the best for the assumed analytic form.

Since the Hartree model assumes that the total wave function, Φ_A , is represented by a simple product of single electron wave functions,

it neglects the pauli principle. Fock improved on the model by requiring that the total wave function be antisymmetric under exchange of any two of the electrons. (See Fock (1930)). The resulting Hartree-Fock model postulates Φ_A to be a Slater determinant of the form

$$\Phi_A = \frac{1}{\sqrt{n!}} \epsilon_{\alpha\beta\cdots\pi} \phi_{\alpha}(1) \phi_{\beta}(2) \cdots \phi_{\pi}(n) \quad (12)$$

where the $\phi(i)$ represents products of electron space and spin functions of the form

$$\phi(i) = \psi(\vec{r}_i) \chi(\sigma_i) \quad (13)$$

By application of the variational principle in the Hartree-Fock model, a Hartree-Fock self-consistent field equation (H-F-EQ), is derived which is analagous to the Hartree equation obtained above. The (H-F) equation is: (See Cyszak (1968).)

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} Y(r) - \epsilon_{n\ell, n\ell} - \frac{\ell(\ell+1)}{r^2} \right] P(n\ell:r) = -2 \int_0^\infty K(n\ell:r,s) P(n\ell:s) ds + \sum_{n' \neq n} \epsilon_{n\ell, n'\ell} P(n'\ell:r) \quad (14)$$

where $Y(r)$ is defined in Eq. (10). The function $K(n\ell:r,s)$ occurring in this equation is defined by the following relations

$$\begin{aligned} u_k(r, r') &= r^{<k}/r^{>k+1} \text{ where } r^{<} \text{ refers to } r \text{ or } r' \\ K_k(n'\ell'; rs) &= P(n'\ell':r) u_k(r,s) P(n'\ell':s) \\ K(n\ell:rs) &= \sum_{\substack{n'\ell' \neq n\ell \\ k'}} K_{k'}(n'\ell'; rs) + \sum_k \alpha_{k\ell} K_k(n\ell:rs) \end{aligned} \quad (15)$$

where the α 's are constants depending on the $P(n\ell:r)$ of interest.

A detailed discussion of the derivation and interpretation of these terms is given by several authors. (In particular the work of Hartree (1957) is useful and the discussion of the Hartree-Fock equation by Cyszak (1968) includes a sample calculation.) For our purpose, it is sufficient to note that the inclusion of exchange couples the equations for the single electron wave functions by introducing the second term on the right-hand side of Eq. (14). Thus, the Hartree-Fock model requires the solution of a coupled set of differential equations and the problem has significantly increased in complexity.

A third model for atomic wave functions which is sometimes used allows for so called "configuration interaction". Recall one of the basic assumptions of the Hartree model is that electrons move independently. Actually the electrons are correlated (see Leighton (1959) or Stevenson (1965)). The correlations are of two types; statistical correlations due to the Pauli Exclusion Principle and coulomb correlations due to the non-central nature of the $1/r_{ij}$ term. The Hartree-Fock model includes statistical correlations by use of determinantal wave functions but ignores coulomb correlations. The coulomb non-central effects together with a spin-spin correlation are discussed in many texts as Russel-Saunders or LS Coupling (see Schiff (1968)). The configuration interaction model is the adoption of an approximate wave function consisting of a linear combination of determinantal wave functions. Since the operators \vec{L}^2 , \vec{S}^2 and Parity commute with the Hamiltonian containing the non-central $1/r_{ij}$ -term, (see Condon (1935)), only those configurations of the same L, S and Parity are included in

the approximate wave function. This model increases the complexity of the calculation of the wave functions still further.

Since each of the atomic models involves a self-consistent calculation, the computations, as might be expected are laborious. The early computations were done by hand, and a compilation of these calculations through 1958 is given by Slater (1960).

In the mid 1950's with the advent of relatively high speed computers Piper (1956) and Vainshtein (1957) made separate attempts to use the Hartree-Fock model to calculate large numbers of atomic wave functions. In 1963 two authors, Herman and Skillman, produced a calculation of all ground state atomic wave functions for all elements. Other calculations have since been made by other authors (as referenced in Cyszak (1968)). These other calculations in general involve two types of procedures; either an analytic procedure or a numerical procedure.

In the analytic procedure the radial wave functions, $P(n_i l_i; r) = P_i(r)$ are taken to have the general form:

$$P_i(r) = \sum_j c_{ij} \left[\frac{(2Z_j)^{2l+2A_j+3}}{(2l+2A_j+2)!} \right] r^{l+A_j+1} e^{-Z_j r} \quad (16)$$

subject to the normalization condition, $\int |P_i(r)| dr = 1$. Here the Z_j 's are screening constants and the A_j 's are the parameters which define the basis functions. A set of P 's are chosen by defining the A_j 's and the best of this set is determined by minimizing $\int \Psi^\dagger H \Psi d\tau$ with respect to variations in the P 's. This determines the Z_j 's. The Hartree-Fock equation is then solved by determining the eigenvectors c_{ij} . (A sample calculation using this technique is discussed by Winterbon (1968)).

In the numerical procedure a straight forward numerical integration of the Hartree-Fock equation is carried out and the $P(nl;r)$ are obtained as tabulated numerical functions. Analytic programs have been developed by Nesbet and Watson (1960), Roothan (1960), Watson and Freeman (1961). Numerical programs such as the Herman and Skillman work, have been also written by Froese (1963) and by Mayers and Hersh (1963). All the above mentioned calculations use the (HF)-model. A program to include configuration interactions has been developed by Mayers and Obrien (1963), and a program to calculate atomic wave functions by use of the Dirac equation has been written by Liberman, Waber, and Cramer (1965).

Since the review of Cyszak (1968), additional wave function calculations have appeared in the literature; Smith (1967) provided numerical solutions to the Dirac equation, Cowan (1967), (1968a), (1968b), using the Herman-Skillman as a starting point has developed calculations of atomic transition probabilities. Other recent works of interest are:

C. (Froese) Fisher (1967), (1968) has expanded her earlier work (see Froese (1963)) to include configuration-interactions; Mayers (1971) with his collaborator Obrien have continued the relativistic wave function work they began in the 60's (see Mayers (1963)); Seaton (1970) has reviewed some of the basic principles of Hartree-Fock calculations.

The work of Herman and Skillman is of interest for the present calculation. Recall that the Hartree-Fock equations Eq. (14) are coupled by the exchange term,

$$\sum_{n' \neq n} \epsilon_{nl, n'l} P(n'l; r) \quad .$$

These equations can be decoupled by means of a simplifying assumption due to Slater (1951), who suggested that the Hartree-Fock exchange potentials for different occupied orbitals could be replaced by an averaged exchange potential obtained from the theory of a free-electron gas.

In a free-electron gas, which is a uniform system, the averaged exchange potential is proportional to the cube root of the electronic charge density (see Slater (1960)),

$$v^{\text{exch}}(r) = -6[3/8\pi \rho(r)]^{1/3}$$

The Slater assumption is that in the atom, which is a non-uniform system, the averaged exchange potential depends only on the local charge density $\rho(r)$.

Collecting all potential energy terms into $V(r)$, the Hartree-Fock equation with the Slater assumption may be written:

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V(r) - \epsilon_{n\ell, n\ell} \right] P(n\ell; r) = 0 \quad (17)$$

The function $V(r)$ is as follows:

$$V(r) = -2Z/r - 2/r \int_0^r \sigma(t) dt - 2 \int_r^\infty \frac{\sigma(t) dt}{t} - 6 \left[\frac{3}{8\pi} \rho(r) \right]^{1/3} \quad (18)$$

$$\sigma(r) = \sum_{n\ell} q_{n\ell} |P(n\ell; r)|^2; \quad \rho(r) = 4\pi r^2 \sigma(r); \quad q_{n\ell} = \left[\begin{array}{c} \text{occupation} \\ \text{number} \end{array} \right]$$

Eq. (17) is the Hartree-Fock Slater (HFS) equation. This approximation decouples the wave equation.

Herman and Skillman wrote a Fortran Program for the IBM 7090 Computer to solve the (HFS) equation and obtain ground state wave functions for all atoms. Their results are given in terms of sets of tabulated orbital radial wave functions for specified configurations. It is

these ground state wave functions (and their eigenenergies) that are used in this calculation. They have been chosen because they have the desired accuracy, can be generated on the available IBM 370/145, and are well-known.

The excited state wave functions which are also needed in the present work were obtained by a modification of the Herman-Skillman program (H-S). Let us note that the decoupling of the wave equations discussed here for the target wave functions is consistent with the cross-section approximations presented in Chapter III (i.e. the approximations to the cross-section do not involve coupled channels). This modification is discussed in Chapter III, Section 2 and the program listing is given in Chapter V, Section 1. From this discussion it will be made clear that the wave functions have been isolated from the cross-section calculation. This has been done so that different wave function programs may be used with the cross-section program used here.

2. Continuum Wave Functions

In addition to the bound state wave functions obtained from the modified Herman-Skillman program, this calculation will require continuum wave functions for use in the calculation of ionization cross-sections. These wave functions will be "coulomb" wave functions. These are the solutions to the problem of an electron moving in a field of charge Z with $1/r$ dependence. The functions are discussed in most standard texts. (For example see Landau (1965) or Schiff (1968)).

The coulomb wave function is a particular form of the confluent hypergeometric function. Since the evaluation of this function requires

elaborate mathematical techniques, two approaches to removing the need for numerically evaluating this function are commonly made in atomic structure calculations.

The first approach is to use bound state wave function of the "analytic" type discussed earlier. This technique allows the evaluation of matrix elements by analytic evaluation of integrals of the form

$$\int_{\alpha r}^{\infty} e^{-\lambda z} z^{\alpha} F(\alpha, \gamma, kz) F(\alpha', \gamma', kz) dz \quad (19)$$

where $F(\alpha, \gamma, kz)$ is the confluent hypergeometric function. See Landau (1958), Peach (1968), and Omidvar (1972).

A second approach is to use numerical bound state wave functions (as we have selected here), and to use some reasonable approximation for the coulomb wave function such as the following one.

The wave function we seek is to describe an electron moving away from a point charge $Z = +1$ with a wave vector \vec{k} and a position vector \vec{r} . This function must satisfy the ionization boundary condition (rather than the scattering condition) of an outgoing "plane" wave and an ingoing "spherical" wave. This system of functions may be obtained from the more common system that are solutions to the scattering problem by applying the time-reversal operator to the scattering solution, (see Landau (1957)). The solutions of interest are of the form

$$\psi_c(\vec{r}) = \frac{1}{4\pi k} \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) e^{-i\delta_{\ell}} R_{k\ell}(r) P_{\ell}(\hat{k} \cdot \hat{r}) \quad (20)$$

where $\delta_{\ell} \equiv \text{ARG } \Gamma(\ell+1-i/k)$, P_{ℓ} is the Legendre Polynomial \hat{i} a unit vector and

$$R_{kl}(r) = \frac{C_{kl}}{(2l+1)!} (2kr) e^{-ikr} {}_1F_2\left(\frac{i}{k} + l + 1, 2l+2, 2ikr\right) \quad (21)$$

where

$$C_{kl} = \frac{2\sqrt{k}}{(1 - \exp(-2\pi/k))} \prod_{s=1}^l (s^2 + 1/k^2)^{1/2} \quad \text{Note } l=0 \Rightarrow \prod = 1 \quad (22)$$

and where ${}_1F_1(a,b,c)$ is the confluent hypergeometric (i.e. Kummer's) function, (see McGuire (1973)). These wave functions have the asymptotic form

$$\psi_c^-(r) \sim \frac{1}{k^2} \sin \left[kr - \frac{l\pi}{2} + \frac{1}{k} \ln(2kr) + \delta_l \right] \quad (23)$$

These are the continuum wave functions used in this calculation.

The evaluation of these wave function in the present work is done using the relation

$$e^{-ikr} {}_1F_1\left(\frac{i}{k} + l + 1, 2l+2, 2ikr\right) = \sum_{n=l+1}^{\infty} A_n^l(k) (kr)^{n-l-1} \quad (24)$$

where

$$A_{l+1}^l(k) = 1 ; \quad A_{l+2}^l(k) = -\frac{1}{k} (l+1)$$

and

$$(n+l)(n-l-1)A_n^l(k) = -(2/k)A_{n-1}^l(k) - A_{n-2}^l(k) \quad (25)$$

This expression is given by Abramowitz (1964). The convergence of this series over the range of l, k, r of interest is such that a maximum of 30 terms is needed to evaluate the wave function.

The criteria for truncation of the sum may be seen in the subroutine FLNR (L,RHO,ETA) listed in Chapter 5, Section 3 of this paper.

III. EXCITATION CROSS-SECTIONS

1. The General Problem

The total electron excitation cross-section, $Q(n_i \ell_i \rightarrow n_f \ell_f)$, we are interested in calculating may be obtained from the scattering amplitude $f(\theta, \phi)$. The general expression is developed below.

The Schrödinger equation for a system of an incident electron with coordinate \vec{r}_0 , and an atomic target with nuclear charge Z and atomic electrons at positions \vec{r}_s is given in atomic units as:

$$\left(\left[-\frac{1}{2} \sum_s \nabla_s^2 - \sum_s \frac{Z}{r_s} + \sum_{st} \frac{1}{r_{st}} \right] + \left[-\frac{1}{2} \nabla_0^2 - \frac{Z}{r_0} + \sum_s \frac{1}{r_{0s}} \right] \right) \Psi(\vec{r}_0, \vec{r}_1 \dots \vec{r}_Z) = E \Psi(\vec{r}_0, \vec{r}_1 \dots \vec{r}_Z) \quad (26)$$

The atomic wave functions are the solutions Ψ_A of the equation:

$$\left[-\frac{1}{2} \sum_s \nabla_s^2 - \sum_s \frac{Z}{r_s} + \sum_{st} \frac{1}{r_{st}} \right] \Psi_A(\vec{r}_1 \dots \vec{r}_Z) = E_A \Psi_A(\vec{r}_1 \dots \vec{r}_Z) \quad (27)$$

Assuming the solutions Ψ_A to be known, they can be chosen as orthonormal basis functions in terms of which the total wave function can be expanded.

$$\Psi(\vec{r}_0, \vec{r}_1 \dots \vec{r}_Z) = \int_P F_P(\vec{r}_0) \Psi_P(\vec{r}_1 \dots \vec{r}_Z) \quad (28)$$

Substituting the expansion into Eq. (26), multiplying the result by $\Psi_F^+(\vec{r}_1 \dots \vec{r}_Z)$ and integrating over $d\vec{r}_1 \dots d\vec{r}_Z$ we find,

$$\left[\nabla^2 + k_F^2 \right] F_F(\vec{r}_0) = 2 \int d\vec{r}_1 \dots d\vec{r}_Z \Psi_F(\vec{r}_1 \dots \vec{r}_Z) V(\vec{r}_0, \vec{r}_1 \dots \vec{r}_Z) \Psi(\vec{r}_0, \vec{r}_1 \dots \vec{r}_Z) \quad (29)$$

where

$$V(\vec{r}_0, \vec{r}_1 \dots \vec{r}_2) = \sum_S \frac{1}{r_{os}} - \frac{Z}{r_0} \quad (30)$$

and

$$k_F^2 = 2(E - E_F);$$

E = total energy of system;

E_F = final energy of atomic target.

Assuming the incoming electron is incident with wave vector \vec{k}_I then our problem requires the asymptotic boundary condition

$$F_F(\vec{r}_0) \sim \exp[i\vec{k}_I \cdot \vec{r}_0] \delta_{FI} + r_0^{-1} \exp[ik_F r_0] f_F(\theta, \phi) \quad (31)$$

Since our equation for $F_F(\vec{r}_0)$ is of the Helmholtz form with a source term, we may write the solution in terms of a Green's function $G(\vec{r}_0, \vec{r}')$

$$F_F(\vec{r}_0) = \exp[i\vec{k}_I \cdot \vec{r}_0] \delta_{FI} + 2 \int d\vec{r}' d\vec{r}_1 \dots d\vec{r}_2 \Psi_F(\vec{r}_1 \dots \vec{r}_2) \\ \times V(\vec{r}', \vec{r}_1 \dots \vec{r}_2) G(\vec{r}_0, \vec{r}') \Psi(\vec{r}_0, \vec{r}_1 \dots \vec{r}_2). \quad (32)$$

Here G satisfies the equation

$$[\nabla^2 + k_F^2] G(\vec{r}_0, \vec{r}') = \delta(\vec{r}_0 - \vec{r}') \quad (33)$$

To satisfy the asymptotic boundary condition Eq. (31), we choose

$$G(\vec{r}_0, \vec{r}') = -\exp[ik_F |\vec{r}_0 - \vec{r}'|] / (4\pi |\vec{r}_0 - \vec{r}'|) \quad (34)$$

Then expanding equation G for large \vec{r}_0 and using

$$k_F |\vec{r}_0 - \vec{r}'| = k_F r_0 - \vec{k}_F \cdot \vec{r}' \quad \text{where} \quad \hat{k}_F = \hat{r}_0$$

we can compare the asymptotic expression for Eq. (32) with that given in Eq. (31) to obtain the result

$$f_F(\theta, \phi) = -\left(\frac{2}{4\pi}\right) \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_Z \exp[-i\vec{k}_F \cdot \vec{r}] \frac{\Psi_F^+(\vec{r}, \vec{r}_1, \dots, \vec{r}_Z) V(\vec{r}, \vec{r}_1, \dots, \vec{r}_Z)}{\Psi(\vec{r}, \vec{r}_1, \dots, \vec{r}_Z)} \quad (35)$$

The differential cross-section is defined to be the flux scattered into the direction (θ, ϕ) per unit incident flux. Since the current density is given by

$$S(\vec{r}, t) = \frac{1}{2i} [\Psi(\vec{r}, t) \nabla \Psi(\vec{r}, t) - \nabla \Psi(\vec{r}, t) \Psi(\vec{r}, t)] \quad (36)$$

it follows from Eq. (31) that the incident flux has the value $(1/2i) * (2k_I)$ while the scattered flux in the direction (θ, ϕ) can be written $(-ik_F) |f(\theta, \phi)|^2 / r^2$. The differential cross-section $dQ/d\Omega$, therefore is given by

$$dQ/d\Omega = (k_F/k_I) |f(\theta, \phi)|^2 \quad (37)$$

The total cross-section, Q , results from the integration of $dQ/d\Omega$ over all angles, i.e.

$$Q = (k_F/k_I) \int d\Omega |f(\Omega)|^2 \quad (38)$$

It can be seen from Eq. (35) that the scattering amplitude involves the total wave function for the incident electron and the atomic target, $\Psi(\vec{r}_0, \vec{r}_1, \dots, \vec{r}_Z)$. But since this total wave function is not known, it is clear that some additional approximation is necessary in order to evaluate an atomic cross-section. Many different approximations have been made in this connection. These can be categorized in terms of those that allow for exchange between the incident electron and the target atom electrons and those that do not. The present calculation computes cross-

sections in three non-exchange approximations and one exchange approximation.

2. Born-Approximation

The simplest approximation is the first Born-Approximation. Here the wave function of the total system is approximated for all $|\vec{r}_0|$ by the correct wave function in the asymptotic region of large $|\vec{r}_0|$, i.e.

$$\Psi(\vec{r}_0, \vec{r}_1, \dots, \vec{r}_2) = \exp[i\vec{K}_I \cdot \vec{r}_0] \Psi(\vec{r}_1, \dots, \vec{r}_2) \quad (39)$$

This approximation leads immediately to the following form for the scattering amplitude;

$$f_{\text{BORN}}(\Omega) = -(1/2\pi) \int d\vec{r} \exp[i(\vec{K}_I - \vec{K}_F) \cdot \vec{r}] V(\vec{r}) \quad (40)$$

where

$$V_{FI}(\vec{r}) = \int d\vec{r}_1 \dots d\vec{r}_2 \Psi_F^*(\vec{r}_1, \dots, \vec{r}_2) \left[\frac{Z}{r} + \sum_s \frac{1}{|\vec{r} - \vec{r}_s|} \right] \Psi_I(\vec{r}_1, \dots, \vec{r}_2) \quad (41)$$

This approximation is most valid for high incident energies.

Classically, at low incident energies, the incoming electron spends more time in the interaction region and, clearly, a free particle description is not accurate.

Using the Bethe integral, (see Schiff (1968)),

$$\int d\vec{r} \exp[i\vec{K} \cdot \vec{r}] / |\vec{r} - \vec{r}_s| = (4\pi/k^2) \exp[i\vec{K} \cdot \vec{r}_s] \quad (42)$$

where $\vec{K} \equiv \vec{K}_I - \vec{K}_F$, the first Born Scattering amplitude can be rewritten

$$f_{\text{BORN}}(\Omega) = -(2/k^2) I_{FI} \quad F \neq I \quad (43)$$

where

$$I_{FI} = \sum_{s=1}^Z \int d\vec{r}_1 \dots d\vec{r}_Z \exp[i\vec{K} \cdot \vec{r}_s] \Psi_F^*(\vec{r}_1 \dots \vec{r}_Z) \Psi_I(\vec{r}_1 \dots \vec{r}_Z) \quad (44)$$

A further simplification results from the following argument.

Recall that a Hartree-Fock wave is an antisymmetrized product wave function of the form

$$\Phi_A = (1/\sqrt{Z!}) \epsilon_{\alpha\beta\dots\pi} \phi_\alpha(1) \phi_\beta(2) \dots \phi_\pi(Z) \quad (45)$$

For the atomic systems considered in the present calculation the assumption is made that the atomic core electrons are unchanged. Then only the wave function of the "active" electron is assumed to differ in the initial and final states of the atom. (The Herman-Skillman program is modified to compute the excited state wave function by solving the HFS equation for the excited state using the self-consistent potential of the ground state configuration.) With this assumption the expression for I_{FI} can be reduced via the relation, (inserting the spin wave function $\chi(\sigma_1 \dots \sigma_Z)$)

$$\begin{aligned} \sum_{s=1}^Z \int d\vec{r}_1 \dots d\vec{r}_Z \Psi_F^*(\vec{r}_1 \dots \vec{r}_Z) \exp[i\vec{K} \cdot \vec{r}_s] \Psi_I(\vec{r}_1 \dots \vec{r}_Z) \chi_F(\sigma_1 \dots \sigma_Z) \chi_I(\sigma_1 \dots \sigma_Z) = \\ \left(\frac{1}{Z!}\right) \sum_{s=1}^Z \epsilon_{\alpha\beta\dots\pi} \epsilon_{\alpha\beta\dots\pi} \int d\vec{r}_1 \dots d\vec{r}_Z \phi_\alpha^*(\vec{r}_1, \sigma_1) \dots \phi_\pi^*(\vec{r}_Z, \sigma_Z) \exp[i\vec{K} \cdot \vec{r}_s] \\ \times \phi_\alpha(\vec{r}_1, \sigma_1) \dots \phi_\pi(\vec{r}_Z, \sigma_Z) \end{aligned} \quad (46)$$

and by use of the following property of the Levi-Chivita symbol;

$$\epsilon_{\alpha\beta\dots\pi} \epsilon_{\alpha\beta\dots\pi} = (Z-1)! \delta_{\pi\pi} \quad (47)$$

(where Z is the number of indices). Consider the p^{th} term of the sum over s in Eq. (44)

$$J_p' = [\epsilon_{\alpha \dots \pi} \epsilon_{\alpha' \dots \pi'} / Z] \int d\vec{r}_1 \dots d\vec{r}_p \dots d\vec{r}_Z \phi_{\alpha}^{(f)}(\vec{r}_1 \sigma_1) \dots \phi_{\delta}^{(f)}(\vec{r}_p \sigma_p) \dots \phi_{\pi}^{(f)}(\vec{r}_Z \sigma_Z) \\ \exp[i\vec{K} \cdot \vec{r}] \phi_{\alpha}^{(i)}(\vec{r}_1 \sigma_1) \dots \phi_{\delta}^{(i)}(\vec{r}_p \sigma_p) \dots \phi_{\pi}^{(i)}(\vec{r}_Z \sigma_Z) = [\epsilon_{\alpha \dots \pi} \epsilon_{\alpha' \dots \pi'} / Z] \\ \int d\vec{r}_1 \phi_{\alpha}^{(f)}(1) \phi_{\alpha}^{(i)}(1) \dots \int d\vec{r}_p \phi_{\delta}^{(f)}(p) \exp[i\vec{K} \cdot \vec{r}_p] \phi_{\delta}^{(i)}(p) \dots \int d\vec{r}_Z \phi_{\pi}^{(f)}(Z) \phi_{\pi}^{(i)}(Z) \quad (48)$$

which, by use of the orthogonality of the ϕ 's reduces to

$$J_p' = \frac{\epsilon_{\alpha \dots \chi \dots \pi} \epsilon_{\alpha' \dots \chi' \dots \pi'}}{Z} \int d\vec{r}_p \phi_{\delta}^{(f)}(\vec{r}_p \sigma_p) \exp[i\vec{K} \cdot \vec{r}_p] \phi_{\delta}^{(i)}(\vec{r}_p \sigma_p) \quad (49)$$

which gives

$$J_p' = \frac{(Z-1)!}{Z!} \delta_{\chi\chi'} \int d\vec{r}_p \phi_{\delta}^{(f)}(\vec{r}_p \sigma_p) \phi_{\delta}^{(i)}(\vec{r}_p \sigma_p) \exp[i\vec{K} \cdot \vec{r}_p] \quad (50)$$

where ϕ_Y^i and ϕ_Y^f denote the initial and final state wave functions of the excited electron. (Since spin does not appear in the Hamiltonian the spin-space and the r -space are decoupled. Let us factor out the spin function and neglect it in further discussions, $\phi(\vec{r}_p, \sigma_p) = \psi(\vec{r}_p) \chi(\sigma_p)$.) Since J_p is clearly independent of p (after integration over \vec{r}_p) the sum in I_{FI} results only in a factor of Z , and the expression for f_{born} reduces to the form,

$$f_{\text{BORN}}(\Omega) = -(2/K^2) \int d\vec{r} \psi_f^*(\vec{r}) \exp[i\vec{K} \cdot \vec{r}] \psi_i(\vec{r}) \quad (51)$$

where the initial and final state single electron wave functions are denoted by ψ_i and ψ_f for clarity. This expression for f_{born} will be of use in discussion of other approximations.

By choosing the z -axis in the \vec{k}_I -direction, so that \vec{K} depends only on the polar angle of \vec{k}_F with respect to \vec{k}_I ,

$$K^2 = K_I^2 + K_F^2 - 2 K_I K_F \cos \Theta; \quad K dK = K_I K_F \sin \Theta d\Theta \quad (52)$$

and the total cross-section can be expressed in the form

$$Q = (K_I/K_F) \int d\Omega |f_{BORN}(\Omega)|^2 = (K_I/K_F) (2\pi) \int_0^\pi |f(\Theta)|^2 \sin\Theta d\Theta \quad (53)$$

$$= (2\pi/K_I^2) \int_{K_{min}}^{K_{max}} |f(K)|^2 K dK ; \quad K_{min}^{max} = K_I \pm K_F$$

If the cross-sections are measured in units πa_B^2 instead of a_B^2 (as is implied by atomic units) this is rewritten

$$Q[\pi a_B^2] = \int_{K_{min}}^{K_{max}} \left(\frac{2}{K_I^2}\right) |f_{BORN}(K)|^2 K dK \quad (54)$$

Since the single electron wave functions are designated by the quantum numbers n & m , while the cross-sections of interest in the present calculation are for transitions of the type $(n\ell \rightarrow n'\ell')$ independent of m , we require for what follows the average of the above expression over m_i and its sum over m_f .

Consider.

$$\sum_{m_i, m_f} \frac{|f(K)|^2}{(2\ell_i + 1)} = \frac{4}{K^4 (2\ell_i + 1)} \sum_{m_i, m_f} \left| \int d\vec{r} \psi_f^*(\vec{r}) \exp[i\vec{K} \cdot \vec{r}] \psi_i(\vec{r}) \right|^2 \quad (55)$$

For the integration over \vec{r} choose the z -axis along the \vec{K} -direction and recall, (Jackson (1962))

$$\exp[iKr \cos\Theta] = \sum_{\lambda} i^{\lambda} [4\pi(2\lambda+1)]^{1/2} j_{\lambda}(Kr) Y_{\lambda 0}(\Omega) \quad (56)$$

Since $\psi_{n\ell m}(\vec{r})$ can be written as $\frac{P_{n\ell}(r) Y_{\ell m}(\Omega)}{r}$

we may write

$$\begin{aligned}
\sum_{m_i, m_f} \left| \int d\vec{r} \Psi_f^+(\vec{r}) \exp[i\vec{K} \cdot \vec{r} \cos \Theta] \Psi_i(\vec{r}) \right|^2 &= \sum_{m_i, m_f} \left| \sum_{\lambda} [4\pi(2\lambda+1)]^{1/2} \right. \\
&\times \left. \int dr P(f) j_{\lambda}(Kr) P(i) \int d\Omega Y_{\ell_f m_f}^+(\Omega) Y_{\lambda 0}(\Omega) Y_{\ell_i m_i}(\Omega) \right|^2 = \\
&\sum_{\lambda, \lambda'} (i)^{\lambda} (-i)^{\lambda'} (4\pi) [(2\lambda+1)(2\lambda'+1)]^{1/2} \int dr dr' \{ P(f) j_{\lambda}(Kr) P(i) \\
&\times P(f') j_{\lambda'}(Kr') P(i') \} \sum_{m_i, m_f} \int d\Omega Y_{\ell_f m_f}^+(\Omega) Y_{\lambda 0}(\Omega) Y_{\ell_i m_i}(\Omega) \int d\Omega' Y_{\ell_f m_f}(\Omega') Y_{\lambda 0}(\Omega') Y_{\ell_i m_i}(\Omega')
\end{aligned} \quad (57)$$

In appendix III the sum involving the angular integrals is evaluated in terms of 3j-symbols. By using the result of that appendix we obtain,

$$\begin{aligned}
\sum_{m_i, m_f} \left| \int d\vec{r} \Psi_f^+(\vec{r}) \exp[i\vec{K} \cdot \vec{r}] \Psi_i(\vec{r}) \right|^2 &= \sum_{\lambda, \lambda'} (i)^{\lambda} (-i)^{\lambda'} (4\pi) [(2\lambda+1)(2\lambda'+1)]^{1/2} \\
&\times \left[\int dr P(i) j_{\lambda}(Kr) P(f) \int dr' P(i') j_{\lambda'}(Kr') P(f') \right] \frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \\
&\times \begin{pmatrix} \ell_f & \ell_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \delta_{\lambda, \lambda'} \Delta(\ell_i, \ell_f, \lambda) = \sum_{\lambda=0}^{\infty} (2\ell_f+1)(2\ell_i+1)(2\lambda+1) \begin{pmatrix} \ell_f & \ell_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\times \left| \int dr P_{n_f \ell_f}(r) j_{\lambda}(Kr) P_{n_i \ell_i}(r) \right|^2 \Delta(\ell_i, \ell_f, \lambda)
\end{aligned} \quad (58)$$

Since the triangle rule, $\Delta(\ell_i, \ell_f, \lambda)$, requires $\lambda(\text{minimum}) = |\ell_i - \ell_f|$ and $\lambda(\text{maximum}) = \ell_i + \ell_f$, we obtain for the required sum the result

$$\begin{aligned}
|f'_{\text{BORN}}(K)|^2 &= \sum_{m_i, m_f} |f_{\text{BORN}}(K)|^2 / (2\lambda_i + 1) = (4/K^4) \sum_{\lambda=\lambda_{\min}}^{\lambda=\lambda_{\max}} (2\ell_f+1)(2\lambda+1) \\
&\times \begin{pmatrix} \ell_f & \ell_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int dr P_{n_f \ell_f}(r) j_{\lambda}(Kr) P_{n_i \ell_i}(r) \right|^2
\end{aligned} \quad (59)$$

Finally the expression for the Born-approximation cross-section

$Q[n_i \ell_i \rightarrow n_f \ell_f]$ reduces to

$$Q[\pi a_B^2] = (2/K^2) \int_{K_I - K_F}^{K_I + K_F} |f'_{\text{BORN}}(K)|^2 K dK \quad (60)$$

This form of $|f'_{\text{BORN}}(K)|^2$ is used in the Born option of the cross-

section program.

3. Bethe Approximation

A simplification of the Born-Approximation is due to Bethe. Recall the expression for the Born scattering amplitude

$$|f_{\text{BORN}}(K)|^2 = \left| -\frac{2}{K^2} \int d\vec{r} \Psi_f^*(\vec{r}) \exp[i\vec{K} \cdot \vec{r}] \Psi_i(\vec{r}) \right|^2 \quad (61)$$

When the z-axis is chosen in the K-direction for the integration and $\exp[iK r \cos\theta]$ is expanded, the following series is obtained

$$|f_{\text{BORN}}(K)|^2 = \left(\frac{4}{K^4} \left[K^2 |(\bar{z})_{if}|^2 + (K^4/4) |(\bar{z}^2)_{if}|^2 + \dots \right] \right) \quad (62)$$

where

$$(\bar{z}^S)_{if} = \int \Psi_f^*(\vec{r}) (r \cos\theta)^S \Psi_i(\vec{r}) d\vec{r} \quad (63)$$

This series converges provided $K a_B \ll 1$ where a_B , the Bohr radius, is the approximate range of the atomic wave functions. For $K a_B \gg 1$ $|f(K)|^2$ is small and contributes negligibly to the excitation cross-section (This is discussed in detail by Mott and Massey (1965) in Chapter XVI of their text.).

Approximating the square of the scattering amplitude by the first non-zero term of this series is the Bethe approximation.

The Legendre polynomial $P_\ell(X)$ has X^ℓ as its highest power of X , the next highest being $X^{\ell-2}$, and so on. This may be seen by the power series solution of the Legendre equation, (Jackson (1962)). Recall that

$$Y_{\ell 0}(\Theta, \Phi) = \sqrt{\frac{(2\ell+1)}{4\pi}} P_{\ell}(\cos\Theta) \quad (64)$$

Hence (see Abramowitz (1964))

$$(\cos\Theta)^S = \sum_{t=0}^S a_t Y_{t0}(\Theta) \quad (65)$$

Using $\Psi_{n\ell m}(\vec{r}) = P_{n\ell}(r) Y_{\ell m}(\Omega)/r$

we may write

$$(Z^S)_{if} = \int_0^{\infty} dr (r)^S P_{n_f \ell_f}(r) P_{n_i \ell_i}(r) \sum_{t=0}^S a_t \langle \ell_f m_f | t 0 | \ell_i m_i \rangle \quad (66)$$

Once again we must average over m_i and sum over m_f :

$$\begin{aligned} \sum_{m_i m_f} |f(k)|^2 / (2\ell_i + 1) &= \left(\frac{4}{K^4} \right) (2\ell_i + 1)^{-1} \sum_{m_i m_f} (K)^{2S} |(Z^S)_{if}|^2 \\ &= \left[\frac{4 K^{2S}}{K^4 (2\ell_i + 1)} \right] \int_0^{\infty} dr (r)^S P_{n_f \ell_f}(r) P_{n_i \ell_i}(r) \int_0^{\infty} dr' (r')^S P_{n_f \ell_f}(r') P_{n_i \ell_i}(r') \quad (67) \end{aligned}$$

$$\times \sum_{t, t'} a_t a_{t'} \sum_{m_i m_f} \langle \ell_f m_f | t 0 | \ell_i m_i \rangle \langle \ell_i m_i | t' 0 | \ell_f m_f \rangle$$

Again using the result of Appendix III we may rewrite the final sum in terms of the 3-j symbol and find:

$$\begin{aligned} |f'_{\text{Bethe}}(k)|^2 &= \frac{4 K^{2S}}{K^4} \left| \int_0^{\infty} dr (r)^S P_{n_i \ell_i}(r) P_{n_f \ell_f}(r) \right|^2 \\ &\quad \times \sum_{t=0}^S \frac{a_t^2 (2\ell_f + 1)}{4\pi} \begin{pmatrix} \ell_i & \ell_f & t \\ 0 & 0 & 0 \end{pmatrix}^2 \Delta(\ell_i \ell_f t) \quad (68) \end{aligned}$$

where s is the first non-zero term in the expansion given in Eq. (62).

The cross-section $Q_{\text{bethe}}(n_i \ell_i \rightarrow n_f \ell_f)$ is:

$$Q_{\text{Bethe}} = \left(\frac{2}{k_i^2}\right) \int_{k_i - k_F}^{k_i + k_F} |f_{\text{Bethe}}(K)|^2 K dK \quad (69)$$

Noting that the K-dependence is isolated, we may write

$$Q_{\text{Bethe}} = \left(\frac{2}{k_i^2}\right) (4) \int_{k_{\min}}^{k_{\max}} \frac{(K)^{2s}}{(K)^3} dK \left| \int_0^\infty dr(r)^s \right. \quad (70)$$

$$\times P_{n_i l_i}(r) P_{n_f l_f}(r) \Big|^2 \sum_{t=0}^s \left(\frac{a_t^2}{4\pi}\right) (2l_f+1) \begin{pmatrix} l_i & l_f & t \\ 0 & 0 & 0 \end{pmatrix}^2 \Delta(l_i l_f t).$$

To evaluate a_t we note the following expression from the power series solution of the Legendre Equation given in Kreyzig (1963)

$$P_l(x) = \sum_{t=0}^l a_t x^t \quad ; \quad a_t = \frac{(2t)!}{2^t (t!)^2} \quad (71)$$

4. Modified Bethe Approximation

The results of the Bethe approximation can be improved for the case of low incident energy electrons by the use of a cut-off procedure developed by Seaton (1955). This approximation is called the Modified Bethe (M.B.) approximation and was first stated as follows:

"The total cross-section Q is the sum of the components Q^l arising from the components of the incident wave with angular momentum $\hbar[l(l+1)]^{1/2}$. For these (components) a limiting value of Q_{\max}^l is set by the requirement of charge conservation (the continuity equation for the optical model). The approximation adopted is to calculate Q^l using the Bethe approximation, to accept the values obtained if $Q_{\text{Bethe}}^l < \frac{1}{2}Q_{\max}^l$ and to put $Q^l = \frac{1}{2}Q_{\max}^l$ if $Q_{\text{Bethe}}^l \geq \frac{1}{2}Q_{\max}^l$."

To clarify further discussion of the approximation it is useful to examine three concepts relating to the approximation.

A. In many standard textbooks, (Shiff (1968), Landau (1957)) the scattering problem is discussed from the position of resolving the initial state into states of definite orbital angular momentum. For elastic scattering by a spherically symmetric potential it may be shown that the scattering amplitude can be decomposed in terms of angular momentum states in the form

$$f(\theta) = (2ik)^{-1} \sum_{l=0}^{\infty} (2l+1) (\exp[2i\delta_l] - 1) P_l(\cos \theta) \quad (72)$$

where δ_l is termed the phase shift.

Inelastic scattering may be described by use of a complex potential (i.e. an optical model potential). Applying the method of partial waves to such a model results in complex phase shift $\delta_l = \alpha_l + i\beta_l$. The elastic, absorption, and total cross-sections may be written in terms of these phase shifts. Introducing $s_l = \exp[2i\delta_l]$ the expression for the absorption cross-section is:

$$Q_{ABS} = \left(\frac{\pi}{k^2} \right)^2 \sum_{l=0}^{\infty} (2l+1) (1 - |s_l|^2) \quad (73)$$

Since $|s_l|^2$ cannot be less than zero the partial absorption cross-section Q^l has a limiting value expressed by the relation

$$Q^l \leq \left[\left(\frac{\pi}{k^2} \right) (2l+1) \right] \equiv Q_{max}^l \quad (74)$$

(If a scattering-matrix formulation of the problem is made, the same condition is contained in the requirement of unitarity of the S-matrix.

Hence Eq. (74) is sometimes referred to as "the unitarity condition".)

B. Recall from earlier discussion, the Bethe approximation is obtained by considering the Born scattering amplitude in the form

$$f_{\text{Born}}(\Omega) = -\left(\frac{2}{K^2}\right) \int d\vec{r} \psi_f^\dagger(\vec{r}) \exp[i\vec{K} \cdot \vec{r}] \psi_i(\vec{r}) \quad (75)$$

and expanding the exponential. In the "exponential statement" of the Bethe approximation, the approximation is said to result from retention of the first non-zero term in the resulting series for the amplitude

$$f(\Omega) = -\left(\frac{2}{K^2}\right) \int d\vec{r} \psi_f^\dagger(\vec{r}) \left(\sum_l \frac{(i\vec{K} \cdot \vec{r})^l}{l!} \right) \psi_i(\vec{r}) \quad (76)$$

Although this is the most common statement of the Bethe approximation, an alternate statement of the approximation can be presented as follows.

Consider the Born scattering amplitude in the form,

$$f_{\text{Born}}(\Omega) = -\left(\frac{1}{2\pi}\right) \int d\vec{r}_0 \exp[i\vec{K} \cdot \vec{r}_0] \left\{ \int d\vec{r}_1 \frac{\psi_f^\dagger(\vec{r}_1) \psi_i(\vec{r}_1)}{|\vec{r}_0 - \vec{r}_1|} \right\} \quad (77)$$

The asymptotic form for the potential

$$V(\vec{r}_0, \vec{r}_1) = 1/|\vec{r}_0 - \vec{r}_1|$$

for large $|\vec{r}_0|$ is obtained from the expression

$$\frac{1}{|\vec{r}_0 - \vec{r}_1|} = \sum_{l=0}^{\infty} \frac{r_1^l}{r_0^{l+1}} P_l(\cos[\hat{r}_0 \cdot \hat{r}_1]); \quad r_1 \text{ is } r_0 \text{ or } r_1 \quad (78)$$

That is

$$V_{\text{Asymp}}(\vec{r}_0, \vec{r}_1) = \lim_{r_0 \rightarrow \infty} \left(\frac{1}{|\vec{r}_0 - \vec{r}_1|} \right) = \sum_{l=0}^{\infty} \frac{r_1^l}{r_0^{l+1}} P_l(\cos[\hat{r}_0 \cdot \hat{r}_1]) \quad (79)$$

The so called "potential statement" of the Bethe approximation results

from approximating the scattering amplitude of Eq. (77) by the first non-zero term in the series resulting from the replacement of the potential by Eq. (79) i.e. the first non-zero term in the series

$$f(\Omega) = -\left(\frac{1}{2\pi}\right) \int d\vec{r}_0 e^{i\vec{k}_0 \cdot \vec{r}_0} \left\{ \sum_{\ell=0}^{\infty} \int d\vec{r}_1 \psi_{\ell}^{\dagger}(\vec{r}_1) \psi_{\ell}(\vec{r}_1) \frac{r_1^{\ell}}{r_0^{\ell+1}} P_{\ell}(\cos[\hat{r}_0 \cdot \hat{r}_1]) \right\}. \quad (80)$$

The equivalence of the exponential statement and the potential statement of the Bethe approximation is demonstrated in Appendix IV.

C. A partial wave analysis of the first Born approximation scattering cross-section, Q_{Born} , is given in Appendix V. The resulting expression for the partial cross-section is:

$$Q_{\text{Born}}^{\lambda'} = (18) (2\ell_f + 1) \frac{K_F}{K_I} \sum_{\ell \ell''} \frac{(2\ell' + 1)(2\ell'' + 1)}{(2\ell + 1)} \begin{pmatrix} \ell_i & \ell_f & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 \quad (81)$$

$$\times \begin{pmatrix} \ell & \ell' & \ell'' \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^{\infty} dr_0 r_0^2 \mathcal{R}_{\ell}^{\text{Born}}(r_0) j_{\ell'}(K_I r_0) j_{\ell''}(K_F r_0) \right|^2$$

where

$$\mathcal{R}_{\ell}^{\text{Born}}(r_0) = \int_0^{\infty} r_i^2 dr_i \frac{r_i^{\ell}}{r_0^{\ell+1}} R_{n_{\ell} \ell_f}(r_i) R_{n_{\ell} \ell_i}(r_i); \quad r_i = \begin{Bmatrix} r_0 \\ r_i \\ r_i \end{Bmatrix} \quad (82)$$

Notice that since the Born expression explicitly contains the term $r <^{\ell}/r >^{\ell+1}$, we may apply the "potential statement" of the Bethe approximation and obtain the Bethe partial cross-section Q_{Bethe}^{ℓ} by the replacement of $\mathcal{R}_{\ell}^{\text{Born}}(r_0)$ with $\mathcal{R}_{\ell}^{\text{Bethe}}(r_0) = \int P(i) P(i) \frac{r_i^{\ell}}{r_0^{\ell+1}} dr_i$ in Eq. (81). Then

$$Q_{\ell}^{\text{Bethe}} = (18) (2\ell_f + 1) \frac{K_F}{K_I} \sum_{\ell' \ell''} \frac{(2\ell' + 1)(2\ell'' + 1)}{(2\ell + 1)} \begin{pmatrix} \ell_i & \ell_f & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 \quad (83)$$

$$\times \begin{pmatrix} \ell & \ell' & \ell'' \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^{\infty} dr_0 (r_0)^2 \mathcal{R}_{\ell}^{\text{Bethe}}(r_0) j_{\ell'}(K_I r_0) j_{\ell''}(K_F r_0) \right|^2$$

Returning to our statement of the Modified Bethe (MB) approximation,

the approximation involves enforcement of the unitarity condition for those Bethe partial cross-sections that violate that condition.

Let l_0 be a value of l such that

$$\begin{aligned} Q_{\text{Bethe}}^l &< \left[\frac{1}{2} Q_{\text{max}}^l = \left(\frac{1}{2K_I^2} \right) (2l+1) \right] \text{ for } (l > l_0) \\ Q_{\text{Bethe}}^l &\geq \left[\frac{1}{2} Q_{\text{max}}^l \right] \text{ for } (l \leq l_0) \end{aligned} \quad (84)$$

Then the Modified Bethe approximation to the cross-section is expressed by the relation

$$Q_{\text{MB}} = \sum_{l=0}^{l_0} \frac{1}{2} Q_{\text{max}}^l + \sum_{l=l_0+1}^{\infty} Q_{\text{Bethe}}^l \quad (85)$$

To compute the cross-section it is convenient to rewrite this expression. Notice the following

$$Q_{\text{Bethe}} = \sum_{l=0}^{l_0} Q_{\text{Bethe}}^l + \sum_{l=l_0+1}^{\infty} Q_{\text{Bethe}}^l \quad (86)$$

or

$$\sum_{l=l_0+1}^{\infty} Q_{\text{Bethe}}^l = Q_{\text{Bethe}} - \sum_{l=0}^{l_0} Q_{\text{Bethe}}^l \quad (87)$$

Also notice

$$\sum_{l=0}^{l_0} \frac{1}{2} Q_{\text{max}}^l = \left(\frac{1}{2K_I^2} \right) \sum_{l=0}^{l_0} (2l+1) = \left(\frac{1}{2K_I^2} \right) (l_0+1)^2 \quad (88)$$

Applying Eq. (87) and Eq. (88) to Eq. (85) we write

$$Q_{\text{MB}} = Q_{\text{Bethe}} + \left(\frac{1}{2K_I^2} \right) (l_0+1)^2 - \sum_{l=0}^{l_0} Q_{\text{Bethe}}^l \quad (89)$$

The computer program of the present calculation computes Q_{Bethe}^l using the "exponential statement", Eq. (76), of the Bethe approximation for use in Eq. (89). Only optically allowed transitions are computed

in this approximation, (i.e. the initial and final states must be s-p, p-d, etc.).

With the restriction to optically allowed transitions the cross-section expressions used in the computer programs are:

$$Q_{\text{Bethe}}^{(\text{optical})} = \left(\frac{8\pi}{3k_z^2} \right) (2l_f + 1) \begin{pmatrix} l_f & l_i & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \ln \left[\frac{k_{\text{max}}}{k_{\text{min}}} \right] \quad (90)$$

$$\times \left\{ \left| \int_0^\infty dr (r) P_{n_f l_f}(r) P_{n_i l_i}(r) \right|^2 \equiv |\langle r \rangle_{if}|^2 \right.$$

$$Q_{\text{Bethe}}^{l'}(\text{optical}) = (72\pi) (2l_f + 1) \begin{pmatrix} l_f & l_i & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 |\langle r \rangle_{if}|^2 \quad (91)$$

$$\times (2l' + 1) \left\{ \begin{pmatrix} 1 & l' & l' - 1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^2(l' - 1) + \begin{pmatrix} 1 & l' & l' + 1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^2(l' + 1) \right\}$$

where

$$J^2(l' \pm 1) \equiv \int_0^\infty dr j_{l'}(k_I r) j_{l' \pm 1}(k_F r) \quad (92)$$

(It is of interest to notice that the scheme of imposing the unitarity condition to cross-section calculations was applied to the Born approximation in 1961, (Seaton (1961)). This resulted in the "Unitarized Born Approximation", since used in calculations found in the literature).

5. The Ochkur Approximation

In our discussion so far we have ignored the indistinguishability of the incident electron from the target electron. These have been "non-exchange" approximations. To examine how exchange effects cross-sections let us return to a general formulation of the problem.

The problem of exchange (i.e. the effects of particle identity

and spin) is discussed in most standard texts in quantum mechanics (e.g. Schiff (1968), Landau (1958), and Gottfried (1966)). For our purposes here let us note

- 1) If the interaction of a system of particles does not depend on spin, then it is possible to write the total wave function for the system as a product of a spatial eigenfunction and a spin eigenfunction.
- 2) Properly symmetrized solutions can be constructed from a general unsymmetrized solution.
- 3) For the case of 2 spin (1/2) - particles there are 3 symmetric (the triplet) and 1 antisymmetric (the singlet) spin eigenfunctions.

For simplicity, let us examine the case of an atom with one valence electron outside a closed shell (i.e. Hydrogen or an Alkali atom).

With our inert-core assumption this is a two electron system. Recall from Chapter III Section 1 Eq. (28) the total unsymmetrized spatial wave function for this system may be written

$$\Psi(\vec{r}_0, \vec{r}_1) = \sum_P F_P(\vec{r}_0) \bar{\Psi}_P(\vec{r}_1) \quad (93)$$

where \vec{r}_0 and \vec{r}_1 are the position vectors of the scattered electron and the valence electron respectively. The summation P in Eq. (93) is over the complete set of states (continuous and discrete) of the atomic target.

Following the procedure of Chapter III Section 1 we find the scattering amplitude (and from it the cross-section) by examining the

asymptotic behavior of the total wave function of the system. Since there are two electrons we require asymptotic forms for the exact unsymmetrized wave function $\Psi(\vec{r}_0, \vec{r}_1)$ when r_0 is large and when r_1 is large. These asymptotic behaviors are:

$$\Psi(\vec{r}_0, \vec{r}_1) \xrightarrow{r_0 \rightarrow \infty} \Psi_I(\vec{r}_1) \exp(i\vec{k}_I \cdot \vec{r}_0) + r_0^{-1} \exp(i\vec{k}_F \cdot \vec{r}_0) f_d(\Omega) \Psi_F(\vec{r}_1) \quad (94)$$

$$\Psi(\vec{r}_0, \vec{r}_1) \xrightarrow{r_1 \rightarrow \infty} \Psi_F(\vec{r}_0) \left[r_1^{-1} \exp(i\vec{k}_F \cdot \vec{r}_1) f_e(\Omega) \right] \quad (95)$$

where f_d and f_e are the direct and exchange scattering amplitude respectively. (Schiff (1968))

Using the singlet and triplet spin wave functions it is clear that the triplet is symmetric and must be multiplied by an antisymmetric spatial wave function ($\Psi(\vec{r}_0, \vec{r}_1) - \Psi(\vec{r}_1, \vec{r}_0)$). Similarly the antisymmetric singlet spin eigenfunction must be multiplied by the symmetric spatial function ($\Psi(\vec{r}_0, \vec{r}_1) + \Psi(\vec{r}_1, \vec{r}_0)$).

The asymptotic form for large values of one of the arguments (because of the symmetrization either will do) say r_0 , is given by

$$\begin{aligned} \Psi(\vec{r}_0, \vec{r}_1) \pm \Psi(\vec{r}_1, \vec{r}_0) \xrightarrow{r_0 \rightarrow \infty} & \exp(i\vec{k}_I \cdot \vec{r}_0) \Psi_I(\vec{r}_1) \\ & + r_0^{-1} \exp(i\vec{k}_F \cdot \vec{r}_0) \left[f_d(\Omega) \pm f_e(\Omega) \right] \Psi_F(\vec{r}_1). \end{aligned} \quad (96)$$

Using the fundamental postulate of quantum mechanics (see Huang (1963)) that all spin states are equally likely to appear in the collision, the differential cross-section must be computed with the symmetric spatial function in 1/4 of the collisions and with the antisymmetric spatial function in 3/4 of the collisions. That is

$$\frac{dQ}{d\Omega} = \frac{1}{4} |f_d(\Omega) + f_e(\Omega)|^2 + \frac{3}{4} |f_d(\Omega) - f_e(\Omega)|^2 \quad (97)$$

With this general understanding of the exchange problem let us now examine an approximation due to Oppenheimer (1928). Analogous to the Born approximation given in Chapter III, Section 2 Eq. (39), Oppenheimer assumed that the exact expression:

$$\Psi(\vec{r}_0, \vec{r}_1) = \int_p \left[F_p(\vec{r}_0) \Psi_p(\vec{r}_1) \pm F_p(\vec{r}_1) \Psi_p(\vec{r}_0) \right] \quad (98)$$

could be approximated

$$\Psi(\vec{r}_0, \vec{r}_1) = \exp(i\vec{k}_i \cdot \vec{r}_0) \bar{\Psi}_p(\vec{r}_1) \pm \exp(i\vec{k}_f \cdot \vec{r}_1) \bar{\Psi}_i(\vec{r}_0) \quad (99)$$

With this approximation it may be shown (see Bates (1950)) that the direct amplitude f_d may be written

$$f_d(\Omega) = - \left(\frac{1}{2\pi} \right) \int d\vec{r}_0 \exp(i[\vec{K}_i - \vec{K}_f] \cdot \vec{r}_0) V_{FI}(\vec{r}_0) \quad (100)$$

where

$$V_{FI}(\vec{r}_0) = \int d\vec{r}_1 \bar{\Psi}_f^\dagger(\vec{r}_1) \frac{1}{|\vec{r}_0 - \vec{r}_1|} \Psi_i(\vec{r}_1) \quad (101)$$

and the exchange amplitude f_e may be written

$$f_e(\Omega) = \left(\frac{1}{2\pi} \right) \iint d\vec{r}_0 d\vec{r}_1 \exp(i\vec{k}_i \cdot \vec{r}_1) \bar{\Psi}_i(\vec{r}_0) \times \frac{1}{|\vec{r}_0 - \vec{r}_1|} \exp(-i\vec{k}_f \cdot \vec{r}_0) \bar{\Psi}_f^\dagger(\vec{r}_1) \quad (102)$$

The extension of the above formulae to the 3 electron case is straight forward but tedious. The 8 spin eigenfunctions for a three

electron system and a derivation of the scattering amplitude for an elastic collision of an electron with a Helium atom is given by Schiff (1968) in Chapter 10 of his book.

The direct and exchange scattering amplitudes for a Helium-like system are:

$$f_d = - \left(\frac{1}{2\pi} \right) \int d\vec{r}_0 \exp(i[\vec{K}_i - \vec{K}_f] \cdot \vec{r}_0) V_{FI}(\vec{r}_0) \quad (103)$$

$$V_{FI}(\vec{r}_0) = \int d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_1, \vec{r}_2) \left[\frac{1}{|\vec{r}_0 - \vec{r}_1|} + \frac{1}{|\vec{r}_0 - \vec{r}_2|} \right] \Psi_I(\vec{r}_1, \vec{r}_2) \quad (104)$$

and

$$f_e = \left(\frac{1}{2\pi} \right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) \exp(-i\vec{K}_f \cdot \vec{r}_1) \\ \times \left[\frac{1}{r_{01}} + \frac{1}{r_{02}} \right] \Psi_I(\vec{r}_1, \vec{r}_2) \exp(i\vec{K}_i \cdot \vec{r}_0) \quad (105)$$

This Born-Oppenheimer approximation to the exchange scattering amplitude, f_e , gives rise to cross-sections which violate the requirement of detail balancing, (i.e. $|H_{FI}|^2 = |H_{IF}|^2$). (see Segre (1965)). In the literature this has been referred to as the "post-prior" discrepancy. It has been shown that this problem arises from the non-orthogonality of the initial and final state wave functions (see Rudge (1965)).

The Ochkur-approximation is an improvement on the Born-Oppenheimer exchange amplitude which removes this discrepancy. In his original work Ochkur (1964) examines the exchange amplitude for Helium, Eq. (105), and notes that "the collision of an electron with an arbitrary atom can

be carried out in a completely analogous manner."

Briefly Ochkur expands the exchange amplitude in a power series in $(1/k_I)$ and retains only the leading term. (This expansion is given in Appendix VI). The resulting approximation to the exchange amplitude is:

$$f_e(\Omega) = \left(\frac{2}{k_I^2}\right) \int d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_1) \exp(i[\vec{K}_I - \vec{K}_F] \cdot \vec{r}_1) \Psi_I(\vec{r}_1, \vec{r}_2) \quad (106)$$

Notice that the "direct" scattering amplitude f_d given in Eq. (103) is the Born scattering amplitude, f_{born} , discussed earlier in Chapter III, Section 2 Eq. (51). Further the Ochkur exchange amplitude, f_e , of Eq. (106) may be written in terms of the Born amplitude as:

$$f_e = \frac{k^2}{k_I^2} f_{\text{born}} \quad (107)$$

where $\vec{K} \equiv \vec{K}_I - \vec{K}_F$

Recall Chapter III, Section 2 that in the present calculation we are making the inert-core-active-electron approximation. In this approximation all target atoms are treated as one valence electron systems. Returning then to our earlier discussion we define

$$\frac{dQ^\pm}{d\Omega} = |f_d(\Omega) \pm f_e(\Omega)|^2 = \left(1 \pm \frac{k^2}{k_I^2}\right) |f_{\text{born}}(\Omega)|^2 \quad (108)$$

and use Eq. (97) to write

$$\frac{dQ}{d\Omega} = \left(\frac{1}{4}\right) \frac{dQ^+}{d\Omega} + \left(\frac{3}{4}\right) \frac{dQ^-}{d\Omega} \quad (109)$$

Then in the usual manner (see Chapter III, Section 2) we may write

$$Q = \frac{k_I}{k_F} \int d\Omega \frac{dQ}{d\Omega} = \left(\frac{2\pi}{k_I^2}\right) \int_{K_{\text{min}}}^{K_{\text{max}}} K dK \frac{dQ}{dK} \quad (110)$$

where

$$\frac{dQ}{dK} = \left(\frac{1}{4}\right) \frac{dQ^+}{dK} + \left(\frac{3}{4}\right) \frac{dQ^-}{dK} \quad (111)$$

Let us again measure cross-sections in units of πa_B^2 . Then the total cross-section is written

$$\begin{aligned} Q_{\text{Ochkur}} &= \left(\frac{2}{K_I^2}\right) \int_{K_{\min}}^{K_{\max}} K dK \left\{ \left(\frac{1}{4}\right) \left(1 + \frac{2K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) + \left(\frac{3}{4}\right) \left(1 - \frac{2K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) \right\} |f_{\text{Born}}(K)|^2 \\ &= \left(\frac{2}{K_I^2}\right) \int_{K_{\min}}^{K_{\max}} K dK \left(1 - \frac{K^2}{K_I^2} + \frac{K^4}{K_I^4}\right) |f_{\text{Born}}(K)|^2. \end{aligned} \quad (112)$$

This is the Ochkur expression used in the present calculation.

Let us note here that it has been observed by Rudge (1965a) that the approximation of Ochkur is "in a certain sense incorrect". Specifically Rudge has shown that the Ochkur expression cannot be obtained from a variational principle. However, the Ochkur approximation does overcome some of the difficulties of the Born-Oppenheimer approximation. For that reason it is still used to incorporate exchange. Rudge himself provides Ochkur calculations in his ionization review paper (see Rudge (1968)). He observes, "The derivation of Ochkur's result is of an ad hoc nature and it is not altogether clear why it yields a marked improvement over the Born-Oppenheimer method."

6. Summary of the Excitation Cross-Section Expressions Used in the Computer Programs.

In summary, the final form of each of the four approximations discussed in this chapter and used in the calculation are given below. Some of the Fortran variable names will also be given for reference.

A) Born

$$Q_{\text{Born}} = \left(\frac{2}{K_I^2} \right) \int_{K_I - K_F}^{K_I + K_F} dK \, K \left| f'_{\text{Born}}(K) \right|^2 \quad (113)$$

where

$$\left| f'_{\text{Born}}(K) \right|^2 = \left(\frac{4}{K^2} \right) \sum_{\lambda=l_i+l_f}^{l_i+l_f} (2l_f+1)(2\lambda+1) \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^\infty dr P_{n_f l_f}(r) j_\lambda(Kr) P_{n_i l_i}(r) \right|^2 \quad (114)$$

B) Bethe

$$Q_{\text{Bethe}} = \left(\frac{8}{K_I^2} \right) \int_{K_I - K_F}^{K_I + K_F} dK \left(\frac{K^{2S}}{K^3} \right) \left| \int_0^\infty dr (r)^3 P_{n_f l_f}(r) P_{n_i l_i}(r) \right|^2 \quad (115)$$

$$\times \sum_{t=l_i+l_f}^S \left(\frac{2l_f+1}{4\pi} \right) \begin{pmatrix} l_i & l_f & t \\ 0 & 0 & 0 \end{pmatrix}^2 \left(\frac{[2t]!}{2^t [t]!} \right)^2$$

C) Modified Bethe

$$Q_{\text{mod. Bethe}}^{(\text{OPTICAL})} = Q_{\text{Bethe}} + \left(\frac{1}{2K_I^2} \right) (l_0+1)^2 - \sum_{l=0}^{l_0} Q_{\text{Bethe}}^l \quad (116)$$

where

$$Q_{\text{Bethe}}^{l'(\text{optical})} = (72) (2l_f+1) \begin{pmatrix} l_i & l_f & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^\infty dr P_{n_f l_f}(r) \right. \quad (117)$$

$$\times \left. \int_0^\infty dr P_{n_i l_i}(r) \right|^2 (2l'+1) \left\{ \begin{pmatrix} 1l'l'-1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^{2(l'-1)} + \begin{pmatrix} 1l'l'+1 \\ 0 & 0 & 0 \end{pmatrix}^2 J^{2(l'+1)} \right\}$$

and where

$$J(l' \pm 1) = \int_0^\infty dr' j_{l'}(K_I r') j_{l' \pm 1}(K_F r') \quad (118)$$

D) Ochkur

$$Q_{\text{Ochkur}} = \left(\frac{2}{K_I^2} \right) \int_{K_I - K_F}^{K_I + K_F} dK \left(1 - \frac{K^2}{K_I^2} + \frac{K^4}{K_I^4} \right) \left| f_{\text{Born}}(K) \right|^2 \quad (119)$$

where $f_{\text{Born}}(K)$ is as given above.

The program listings and a discussion are given in Chapter V, Section 2. Some of the Fortran names used for the variables in the

above expressions are:

$$Q \rightarrow \text{SIG}$$

$$K_x \rightarrow \text{XIN}$$

$$K_F \rightarrow \text{XF}$$

$$l_i \rightarrow \text{L1}$$

$$l_f \rightarrow \text{L2}$$

$$P_{n_i l_i} \rightarrow \text{PF}$$

$$K \rightarrow \text{X}$$

$$r \rightarrow \text{Y}$$

$$\lambda \rightarrow \text{LAM}$$

$$J \rightarrow \text{F}$$

$$j_x \rightarrow \text{BJ}$$

$$\begin{pmatrix} l_1 l_2 l_3 \\ 0 0 0 \end{pmatrix} \rightarrow \text{TJ}(\text{L1}, \text{L2}, \text{L3})$$

$$\left| \int_0^\infty dr P_{n_i l_i}(r) j_\lambda(\kappa r) P_{n_f l_f}(r) \right|^2 \rightarrow \text{RDINT}(\text{BJ}, \text{LAM}, \text{X})$$

It may be shown (Gottfried (1966)) that for a potential $U(r)$ the criterion for validity of the Born approximation is

$$\frac{1}{\kappa_i} \left| \int_0^\infty \exp(i\kappa_i r) \sin(\kappa_f r) U(r) dr \right| \ll 1$$

Gottfried argues that for a neutral atom of charge Z (in some cases an effective charge) this condition is equivalent to

$$Z \sqrt{E_H} \ll \sqrt{E}$$

where E_H is the Rydberg. An upper limit of E is set by the fact that we are considering non-relativistic electrons and therefore $E \ll mc^2$. Hence the region of validity for the Born approximation in eV is

$$(Z)(3.1) \ll \sqrt{E} \ll 7.1 \times 10^2, \text{ or } Z \ll 200$$

Gottfried notes that "the Born approximation actually leads to considerably more accurate inelastic cross-sections at low energies than one would surmise from this inequality."

The Bethe approximation assumes the above condition is satisfied and furthermore assumes that

$$\left[(\kappa_3)_{\text{IF}}^s / s! \right] / \left[(\kappa_3)_{\text{IF}}^{s-1} / (s-1)! \right] \ll 1$$

s is the power of the first non-zero term in the Bethe series (Eq. 62).

The Ochkur approximation must satisfy the Born criterion, and the Modified Bethe approximation must satisfy both the Born and Bethe criteria.

The expected validity of the results for the specific calculations of this paper will be given after some of the results are considered.

IV. IONIZATION CROSS-SECTION

1. Relationship to Excitation Expressions

The problem of electron collisions with neutral atoms causing ionization is both similar and dramatically different from the problem of excitation. It is similar insofar as we can state ionization as "excitation to the continuum". Having noted this, much of the earlier discussion of the excitation problem (and many of the expressions derived) may be applied to ionization, but with caution.

The ionization problem is dramatically different for two reasons. First, the continuum state wave functions only have specific states associated with specific wave-vectors \vec{k}_e . Therefore, an ionization cross-section is excited to a state with specific direction. Second, the electron that is ionized (secondary electron) is indistinguishable from the scattering electron and this must be accounted for in the computation.

2. The Born-Coulomb Approximation

The most commonly used approximation to the cross-section for electron impact ionization of neutral atoms is the Born-Coulomb approximation. This is an approximation of the cross-section by the Born-approximation derived earlier, with the final state of the atom (the ionized electron) described by a Coulomb wave.

Consider the system of an electron with a wave vector \vec{k}_I incident on an atom described by the atomic wave function ψ_i . In this system the electron is scattered into a direction (Ω_F) with a wave vector k_F and the

atom is ionized, emitting a secondary electron into a direction (Ω_e) with a wave vector \vec{k}_e . Let us derive the cross-section for this collision.

Using the Born approximation (i.e. describe the primary electron by the plane waves $\exp(i\vec{k}_I \cdot \vec{r})$ and $\exp(-i\vec{k}_F \cdot \vec{r})$ and the inert-core approximation recall:

$$\frac{dQ}{d\vec{k}_e} [\pi\theta_p] = \left(\frac{2}{K_I^4} \right) \int_{K_I - K_F}^{K_I + K_F} K dK |f_{\text{Born}}(\vec{K}, \vec{k}_e)|^2 \quad (120)$$

where

$$f_{\text{Born}}(\vec{k}_e, K) = \left(\frac{2}{K^2} \right) \int d\vec{r} \psi_f^\dagger(\vec{k}_e, \vec{r}) \exp(i\vec{K} \cdot \vec{r}) \psi_i(\vec{r}) \quad (121)$$

Let us assume the atomic wave functions are of the form:

$$\psi_i(\vec{r}) = R_{n_i \ell_i}(r) Y_{\ell_i m_i}(\Omega_r) \quad (122)$$

$$\psi_f(\vec{k}_e, \vec{r}) = \sum_{\ell_e=0}^{\infty} R_{\ell_e}(k_e, r) P_{\ell_e}(\hat{k}_e \cdot \hat{r}) \quad (123)$$

To integrate Eq. (121) choose the z-axis along the \vec{k} -direction and recall

$$\exp(ikr \cos \theta) = \sum_{\lambda=0}^{\infty} i^\lambda [4\pi(2\lambda+1)]^{1/2} j_\lambda(kr) Y_{\lambda 0}(\Omega_r) \quad (124)$$

Using the addition theorem to write

$$\psi_f(\vec{k}_e, \vec{r}) = \sum_{\ell_e, m_e} \left\{ \frac{4\pi}{(2\ell_e+1)} R_{\ell_e}(k_e, r) Y_{\ell_e m_e}^\dagger(\Omega_{k_e}) \right\} Y_{\ell_e m_e}(\Omega_r) \quad (125)$$

then Eq. (121) may be expanded as

$$\begin{aligned}
f_{\text{Born}}(\vec{\kappa}_e, \kappa) &= -\left(\frac{2}{\kappa^2}\right) \sum_{l_e m_e \lambda} \left\{ \left(\frac{4\pi}{2l_e+1} \right) i^\lambda [4\pi(2\lambda+1)]^{1/2} \equiv c(l_e, \lambda) \right\} \\
&\times Y_{l_e m_e}(\Omega_{\kappa_e}) \left\{ \int d\Omega_r Y_{l_e m_e}^\dagger(\Omega_r) Y_{\lambda 0}(\Omega_i) Y_{l_i m_i}(\Omega_r) \equiv \langle l_e m_e | \lambda 0 | l_i m_i \rangle \right\} \\
&\times \left\{ \int_0^\infty r^2 dr R_{l_e}(\kappa_e, r) j_\lambda(\kappa r) R_{l_i m_i}(r) \equiv \mathcal{R}(l_e, \lambda, l_i) \right\} \\
&= -\left(\frac{2}{\kappa^2}\right) \sum_{l_e m_e \lambda} c(l_e, \lambda) Y_{l_e m_e}(\Omega_{\kappa_e}) \langle l_e m_e | \lambda 0 | l_i m_i \rangle \mathcal{R}(l_e, \lambda, l_i).
\end{aligned} \quad (126)$$

To find the cross-section we require

$$\begin{aligned}
|f_{\text{Born}}(\vec{\kappa}_e, \vec{\kappa})|^2 &= \left(\frac{4}{\kappa^4}\right) \sum_{l_e m_e \lambda} \sum_{l_e m_e \lambda} c(l_e, \lambda) c^\dagger(l_e, \lambda) Y_{l_e m_e}(\Omega_{\kappa_e}) Y_{l_e m_e}^\dagger(\Omega_{\kappa_e}) \\
&\times \langle l_e m_e | \lambda 0 | l_i m_i \rangle \langle l_i m_i | \lambda 0 | l_e m_e \rangle \mathcal{R}(l_e, \lambda, l_i) \mathcal{R}(l_e, \lambda, l_i).
\end{aligned} \quad (127)$$

This would allow us to calculate the cross-section $\frac{dQ}{d\vec{\kappa}_e}$ for the collision. But the total ionization cross-section would be for all allowed values of the secondary wave-vector. That is

$$Q_{\text{Born}}^{\text{IONIZATION}} = \int_{\frac{Q_{\text{th}}}{\kappa_e}} d\vec{\kappa}_e \frac{dQ}{d\vec{\kappa}_e} = \int_0^{\kappa_e^{\text{max}}} \kappa_e^2 d\kappa_e \int d\Omega_{\kappa_e} \frac{dQ}{d\vec{\kappa}_e} \quad (128)$$

where for a given initial state of the atom and a given incident energy of the primary electron κ_e^{max} is determined by the conservation of energy for the condition of the primary electron at rest. That is,

$$E_e^{\text{max}} = E_i - E_{\text{ionization}}.$$

We may rewrite Eq. (128) as

$$Q_{\text{Born}}^{\text{Ion.}} = \left(\frac{2}{\kappa_i^2}\right) \int_0^{\kappa_e^{\text{max}}} \kappa_e^2 d\kappa_e \int d\Omega_{\kappa_e} \int_{\kappa_{\text{min}}}^{\kappa_{\text{max}}} \kappa d\kappa |f_{\text{Born}}(\vec{\kappa}_e, \kappa)|^2 \quad (129)$$

Using Eq. (127) and noting

$$\int d\Omega_{\kappa_e} Y_{l_e m_e}(\Omega_{\kappa_e}) Y_{l_e m_e}^+(\Omega_{\kappa_e}) = \int_{l_e} \int_{m_e} \quad (130)$$

we can sum over $l_e m_e$ and write

$$|f(\kappa, \kappa_e)|^2 = \int d\Omega_{\kappa_e} |f(\kappa, \vec{\kappa}_e)|^2 = \left(\frac{4}{K^4}\right) \sum_{\lambda \Lambda l_e m_e} c(l_e \lambda) c^+(l_e \Lambda) \times \langle l_e m_e | \lambda 0 | l_i m_i \rangle \langle l_i m_i | \Lambda 0 | l_e m_e \rangle R(l_e \lambda l_i) R(l_e \Lambda l_i) \quad (131)$$

averaging over m_i we write

$$|f'(\kappa, \kappa_e)|^2 = \sum_{m_i} \frac{|f(\kappa, \kappa_e)|^2}{(2l_i + 1)} = \left(\frac{4}{K^4}\right) \sum_{\lambda \Lambda l_e} c(l_e \lambda) c^+(l_e \Lambda) \times R(l_e \lambda l_i) R(l_e \Lambda l_i) \sum_{m_i m_e} \langle l_e m_e | \lambda 0 | l_i m_i \rangle \langle l_i m_i | \Lambda 0 | l_e m_e \rangle \quad (132)$$

With Appendix III we can write

$$\sum_{m_i m_e} \langle l_e m_e | \lambda 0 | l_i m_i \rangle \langle l_i m_i | \Lambda 0 | l_e m_e \rangle = \frac{(2l_e + 1)(2l_i + 1)}{4\pi} \times \begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0 \end{pmatrix} \delta_{\lambda \Lambda} \Delta(l_i l_e \lambda) \quad (133)$$

summing over Λ in Eq. (132) we write

$$|f'(\kappa, \kappa_e)|^2 = \left(\frac{4}{K^4}\right) \sum_{\lambda l_e} |c(l_e \lambda)|^2 |R(l_i \lambda l_e)|^2 \frac{(2l_e + 1)}{4\pi} \begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \\ = \left(\frac{4}{K^4}\right) \sum_{\lambda l_e} \begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \left| \int_0^\infty dr r^2 R_{l_e}(\kappa_e, r) j_\lambda(\kappa r) R_{l_i l_i}(r) \right|^2 \quad (134) \\ \times \left\{ \left(\frac{2l_e + 1}{4\pi} \right) \left(\frac{4\pi}{2l_e + 1} \right)^2 [4\pi(2\lambda + 1)] = (4\pi)^2 \left(\frac{2\lambda + 1}{2l_e + 1} \right) \right\}$$

In summary, the total ionization cross-section in the Born-

Approximation is:

$$Q_{\text{BORN}}^{\text{ION}} = \int_0^{\kappa_e^{\text{max}}} \kappa_e^2 d\kappa_e \frac{dQ}{d\kappa_e} \quad (135)$$

$$\frac{dQ}{d\kappa_e} = \left(\frac{2}{K^2}\right) \int_{K_I - K_F}^{K_I + K_F} K dK |f'_{\text{BORN}}(\kappa, \kappa_e)|^2 \quad (136)$$

$$|f'_{Born}(K, K_e)|^2 = \left(\frac{64\pi^2}{K^4} \right) \sum_{\lambda, l_e} \begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2\lambda+1)}{(2l_e+1)} \left| \int_0^\infty r^2 dr P_{l_e}(K_e, r) j_\lambda(Kr) P_{n_i, l_i}(r) \right|^2 \quad (137)$$

where K_e^{\max} in atomic units is

$$K_e^{\max} = \sqrt{(K_i^2 - 2I)} \quad I = \text{Ionization Energy}$$

However, as mentioned earlier we must account for the secondary electron being indistinguishable from the primary electron. As discussed by Rudge (1968) this may be approximated by setting E_e^{\max} equal to $E_e^{\max}/2$.

Then

$$K_e^{\max} = \sqrt{2(K_i^2 - 2I)} \quad (138)$$

3. The Expression Used in the Computer Programs.

In summary, the expressions used in the calculation are given below.

Some of the Fortran variable names are also given.

$$Q_{Born}^{ION} = \int_0^{K_e^{\max}} K_e^2 dK_e \frac{dQ}{dK_e} \quad (139)$$

$$\frac{dQ}{dK_e} = \left(\frac{2}{K_i^2} \right) \int_{K_i - K_e}^{K_i + K_e} K dK |f'_{Born}(K, K_e)|^2 \quad (140)$$

$$|f'_{Born}(K, K_e)|^2 = \left(\frac{64\pi^2}{K^4} \right) \sum_{\lambda=l_i-l_e}^{l_i+l_e} \begin{pmatrix} l_i & l_e & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{(2\lambda+1)}{(2l_e+1)} \left| \int_0^\infty dr P_{l_e}(K_e, r) j_\lambda(Kr) P_{n_i, l_i}(r) \right|^2 \quad (141)$$

The program listing and discussion is presented in Chapter V, Section 3.

Some of the Fortran variable names are:

$K_e \rightarrow \text{KAPA}$

$\pi \rightarrow \text{PI}$

$\lambda_e \rightarrow \text{L2}$

$P_{\lambda e}(K_e, r) \rightarrow \text{PF}$

V. COMPUTER PROGRAMS

In this chapter the programs themselves will be presented. For each of the three programs used in the calculation (HFSWF, EXCSCT, IONCST) a program listing is given, and some details of the program are discussed. The information on how to run the program is given in Appendix VII--User Manual.

1. Wave Function Program

This program, named HFSWF, is a self-consistent field calculation of radial atomic wave functions. The program consists of a main routine and a subroutine SCHEQ.

a) Listing

PROGRAM HFSWF(INPUT)

```
=====
*
*           * * *   HFSWF   * * *
*
* A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER
* NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT.
* ITERATION NUMBER, MEASURE OF SELF-CONSISTENCY AND
* ATOMIC NUMBER Z ARE ALWAYS PRINTED ON=LINE.
*
* IF KEY=0 NORMALIZED NUMERICAL ATOMIC POTENTIAL IS
* READ IN AS 110 VALUES, EVERY 4TH MESH POINT 1 TO 437.
*
* IF KEY=1 COMPLETE ATOMIC POTENTIAL IS READ IN (437PT)
* IF KEY=2 EXTRAPOLATE STARTING POTENTIAL
*
* MAXIT=MAXIMUM NO.OF ITERATIONS(MAXIT=0 IMPLIES 20).
*
* IF KUT=0, MODIFIED H-F-S POTENTIAL IS USED IN WV.=EQ.
* IF KUT=1, UNMODIFIED H-F-S POTENTIAL IS USED IN WV.=EQ.
*
* IF NOCOPY=0, ACTIVE ELECTRON WAVE FUNCTIONS ARE PUNCHED
* IF NOCOPY=1 ALL WV. FNCTS. AND SELF-CONSISTENT
* POTENTIAL ARE PRINTED ON=LINE.
=====
```

```
*
*           PROGRAM AND SUBROUTINES
*           ORIGINALLY WRITTEN BY
* SHERWOOD SKILLMAN, RCA-LAB, PRINCETON NJ, SPR 1961
*           MODIFIED BY
* (1) F. HERMAN, RCA-LAB, PRINCETON NJ, SUMMER 1961
* (2) R. KORTUM, LCKHEED RSRCH-LAB, PALO ALTO, SM 1962
* (3) T. GREENE, UNIV. OF TOLEDO, TOL. OHIO, FALL 1971.
* *****
```

```
DIMENSION X(521), RSCORE(521), RUINL1(521), RU2(521), RU(521), NNL
1Z(24), R(521), RSVALE(521), RUENL1(521), RU3(521), XI(521), WWNL(2
24), V(521), RSATOM(521), RUINL2(521), XNUM(521), XJ(521), NKKK(24)
3, EE(24), RUEXCH(521), RUENL2(521), DENM(521), SNL(10,521), SNLO(5
421), A(4,5)
```

```
COMMON V, SNLO, R, RSCORE, RSVALE, RU, RUEXCH, XI, XJ, RSATOM, SNL, RUINL1, RU
1FNL1, RUINL2, RUENL2, RU2, RU3, NNLZ, WWNL, NKKK, EE, A
EQUIVALENCE (RSCORE, XNUM), (RSVALE, DENM), (GQ, RSATOM)
NFILES=0
```

1 CONTINUE

READ HEADING CARD.

```
READ (5,138)
WRITE (6,138)
```

READ CONTROL CARDS AND INPUT POTENTIALS. CALCULATE TRIAL POTENTIAL

NCARDS=90

PRINT 132, KEY

```
READ (5,131) KEY, TOL, THRESH, MESH, IPRATT, MAXIT, NOCOPY, KUT, IP, IM, IR,
1ID, DEFOLT, JE
```

```

      IF (DEFOLT) 2,2,3
2  KEY=0
   TOL=.001
   TRESH=.00001
   MESH=441
   IPRATT=1
   MAXIT=20
   NOCOPY=1
   KUT=0
   IP=6
   IM=6
   IR=5
   IC=7
   JE=1
   GO TO 5
3  IF (MAXIT) 4,4,5
4  MAXIT=20
5  CONTINUE
   NBLOCK=(MESH)/40

C
C   CONSTRUCT X MESH AND R MESH
C
   I=1
   X(I)=0.0
   R(I)=0.0
   DELTAX=0.0025
   DO 7 J=1,NBLOCK
   DO 6 K=1,40
   I=I+1
6  X(I)=X(I-1)+DELTAX
7  DELTAX=DELTAX+DELTAX
   IF (KEY=1) 9,10,8
8  READ (IR,129) (RU2(M),M=1,441)
   READ (IR,129) (RU3(M),M=1,441)
   ZE2=-RU2(1)/2.0
   ZE3=-RU3(1)/2.0
   GO TO 11

C
C   READ IN ATOMIC POTENTIAL
C
9  READ (IR,124) (RU2(M),M=1,437,4)
   GO TO 11
10 READ (IR,129) (RU3(M),M=1,441)
   ZE3=-RU3(1)/2.0
11 READ (IR,125) Z,NCORES,NVALES,ION
   IF (Z) 120,1,12
12 NFILES=NFILES+1
   AZ=Z
   IZ=Z
   NCSPVS=NCORES+NVALES
   C=0.88534138/Z**(1.0/3.0)
   TWOION=ION+ION
   ZZZ=ION+1
   TWOZZZ=ZZZ+ZZZ
   DO 13 I=2,MESH
13 R(I)=C*X(I)
   READ (IR,127) (NNLZ(I),WWNL(I),EE(I),I=1,NCSPVS)
   WWW=0.0
   DO 14 I=1,NCSPVS

```



```

14 WWW=WWW+WWNL(I)
   IF (ABS(Z+1.0-WWW-ZZZ)=0.001) 16,15,15
15 PRINT 126, WWW,ZZZ,Z,NCORES,NVALES,NCSPVS
   CALL EXIT
16 CONTINUE
   IF (KEY=1) 21,26,17

```

C

C

C

```

CONSTRUCT ATOMIC POTENTIAL

```

```

17 IF (ABS(ZE3-ZE2-Z+ZE3)=0.001) 19,19,18
18 WRITE (IP,139) Z,ZE2,ZE3
   CALL EXIT
19 DO 20 I=1,441
   RU(I)=RU3(I)+RU3(I)-RU2(I)
20 CONTINUE
   GO TO 31
21 TWOZ=Z+Z
   DO 22 I=1,437,4
22 RU(I)=-RU2(I)*TWOZ
   RU(441)=RU(437)
   RU(445)=RU(437)
   M=9
   DO 25 I=1,437,4
   M=M+1
   IF (M) 23,24,24
23 RU(I+1)=(22.0*RU(I)+11.0*RU(I+4)-RU(I+8))/32.0
   RU(I+2)=(10.0*RU(I)+15.0*RU(I+4)-RU(I+8))/24.0
   RU(I+3)=(6.0*RU(I)+27.0*RU(I+4)-RU(I+8))/32.0
   M=9
   GO TO 25
24 RU(I+1)=(21.0*RU(I)+14.0*RU(I+4)-3.0*RU(I+8))/32.0
   RU(I+2)=(3.0*RU(I)+6.0*RU(I+4)-RU(I+8))/8.0
   RU(I+3)=(5.0*RU(I)+30.0*RU(I+4)-3.0*RU(I+8))/32.0
25 CONTINUE
   GO TO 31
26 IF (ABS(ZE3-Z)=0.001) 27,27,29
27 DO 28 I=1,441
   RU(I)=RU3(I)
28 CONTINUE
   GO TO 31
29 ZOZ=Z/ZE3
   DO 30 I=1,441
   RU(I)=RU3(I)*ZOZ
30 CONTINUE
31 V(I)=-9.5E35
   M=MINO(441,MESH)
   IF (KUT) 32,37,32
32 DO 33 I=1,M
33 V(I)=RU(I)/R(I)
   IF (MESH=M) 34,34,36
34 DO 35 I=442,MESH
35 V(I)=-TWOION/R(I)
36 LIMIT=M
   ICUT=MESH
   IC=MESH
   GO TO 47
37 CONTINUE
   ICUT=0
   DO 42 I=2,M

```

```

      IF (ICUT) 38,38,40
38  IF (TWOZZZ+RU(I)) 41,41,39
39  ICUT=I
40  V(I)=TWOZZZ/R(I)
      GO TO 42
41  V(I)=RU(I)/R(I)
42  CONTINUE
      IF (ICUT) 43,43,44
43  ICUT=M
44  LIMIT=ICUT
      IF (MESH=M) 47,47,45
45  CONTINUE
      DO 46 I=442,MESH
46  V(I)=TWOZZZ/R(I)
47  CONTINUE
      DELTA=1000000.
      NITER=0
      NONMON=3
      IPRSW=0
      PRINT 133

```

C
C
C

START ITERATION

```

48  MCARDS=90
      IF (MAXIT=NITER) 49,51,51
49  CONTINUE
      WRITE (IP,140)
      DO 50 I=1,MESH,5
      WRITE (IP,141) I,X(I),RU3(I),RUINL1(I),RUENL1(I),RUINL2(I),RUENL2(
      I),RU(I)
50  CONTINUE
      GO TO 11
51  DO 52 I=1,MESH
      RSCORE(I)=0.0
52  RSVALE(I)=0.0

```

C
C
C
C

SOLVE SCHROEDINGER EQUATION FOR EACH ORBITAL IN TURN
CALCULATE CORE AND VALENCE ELECTRONIC DENSITIES

```

      DO 59 M=1,NCSPVS
      E=EE(M)
      NN=NNLZ(M)/100
      LAM=NNLZ(M)/10=10*NN
      XL=LAM

```

C
C
C

CALL SCHEQ (Z,E,LAM,NN,KKK,MESH,C,THRESH)

```

      IF (M=NCORES) 53,53,55
53  DO 54 I=1,KKK
54  RSCORE(I)=RSCORE(I)+WWNL(M)*SNLO(I)**2
      GO TO 57
55  DO 56 I=1,KKK
56  RSVALE(I)=RSVALE(I)+WWNL(M)*SNLO(I)**2
57  DO 58 I=1,KKK
58  SNL(M,I)=SNLO(I)
      NKKK(M)=KKK
      MCARDS=MCARDS+2+((KKK=1)/40)*8
59  EE(M)=E

```

C

```

C      CALCULATE TOTAL ELECTRONIC DENSITY AND ATOMIC EXCHANGE POTENTIAL
C
      DO 60 I=1,MESH
      RSATOM(I)=RSCORE(I)+RSVALE(I)
60    RUEXCH(I)=6.0*((3.0*R(I)*RSATOM(I))/315.82734)**(1.0/3.0)
C
C      CALCULATE ATOMIC COULOMB POTENTIAL
C
      A1=0.0
      ASUM=0.0
      B1=0.0
      BSUM=0.0
      H=0.0025*C
      I=1
      XI(1)=0.0
      XJ(1)=0.0
      DO 62 J=1,NBLOCK
      DO 61 K=1,40
      I=I+1
      A2=RSATOM(I)/2.0
      A1=A1+A2
      B2=RSATOM(I)/(2.0*R(I))
      B1=B1+B2
      XI(I)=ASUM+A1*H
      XJ(I)=BSUM+B1*H
      A1=A1+A2
61    B1=B1+B2
      ASUM=XI(I)
      BSUM=XJ(I)
      A1=A2
      B1=B2
62    H=H+H
      DO 63 I=1,MESH
      XI(I)=2.0*Z+2.0*(XI(I)+R(I)*(XJ(MESH)-XJ(I)))
      XJ(I)=XI(I)+RUEXCH(I)
63    CONTINUE
      DO 64 I=1,MESH
      RUINL1(I)=RUINL2(I)
      RUFNL1(I)=RUFNL2(I)
      RUINL2(I)=RU(I)
64    RUFNL2(I)=XJ(I)
      NITER=NITER+1
      PDELTA=DELTA
      DELTA=0.0
      DO 66 I=1,LIMIT
      SNLO(I)=RU(I)-XJ(I)
      XI(I)=ABS(SNLO(I))
      IF (XI(I)=DELTA) 66,66,65
65    DELTA=XI(I)
      IDELTA=I
66    CONTINUE
      PRINT 128, NITER,Z,DELTA,IDELTA,X(IDELTA),ICUT,X(ICUT)
C
C      TEST SELF-CONSISTENCY OF ATOMIC POTENTIAL.
C
      IF (DELTA=TOL) 106,67,67
C
C      IF SCF CRITERION NOT SATISFIED, CALCULATE NEXT TRIAL POTENTIAL
C

```

```

67 IF (IPRSW) 68,68,73
68 DO 69 I=2,LIMIT
69 RU(I)=0.5*(RU(I)+XJ(I))
   IF (MESH=LIMIT) 72,72,70
70 RUZM=XJ(MESH)
   RATIO=(RUZM-RU(LIMIT))/(RUZM-XJ(LIMIT))
   DO 71 I=LIMIT,MESH
71 RU(I)=RUZM-RATIO*(RUZM-XJ(I))
   LIMIT=MESH
72 IPRSW=IPRATT
   GO TO 93
73 CONTINUE
   IF (NONMON) 68,68,74
74 IF (PDELTA=DELTA) 75,75,76

C
C   IF DELTA IS NOT MONOTONIC DECREASING FOUR TIMES, BYPASS
C   PRATT IMPROVEMENT SCHEME
C
75 NONMON=NONMON+1
   IF (NONMON) 68,68,76
76 ALPH=0.5

C
C   PRATT IMPROVEMENT SCHEME
C
   DO 84 I=2,ICUT
   XNUM(I)=RUINL1(I)*RUFNL2(I)-RUINL2(I)*RUFNL1(I)
   DENM(I)=RUFNL2(I)-RUFNL1(I)-RUINL2(I)+RUINL1(I)
   IF (ABS(DENM(I)/RUINL2(I))-0.0001) 77,77,78
77 CONTINUE
   ALPH=0.5
   GO TO 83
78 ALPH=(XNUM(I)/DENM(I)-RUFNL2(I))/SNLO(I)
   IF (ALPH) 79,82,80
79 ALPH=0.0
   GO TO 83
80 IF (0.5=ALPH) 81,82,82
81 ALPH=0.5
82 CONTINUE
83 XI(I)=ALPH
84 CONTINUE
   IPRSW=IPRSW+1
   IF (KUT) 87,85,87
85 CONTINUE
   IC=ICUT+20
   IC1=ICUT+1
   ADEL=XI(ICUT)/20.
   DO 86 I=IC1,IC
   XI(I)=XI(I-1)-ADEL
86 XJ(I)=XI(I)
87 CONTINUE
   XJ(1)=0.5
   XJ(2)=XI(2)
   ASUM=XI(2)+XI(3)+XI(4)+XI(5)
   DO 88 I=3,ICUT
   XJ(I)=ASUM*0.2
88 ASUM=ASUM-XI(I-2)+XI(I+3)
   IF (KUT) 91,89,91
89 CONTINUE
   IC1=IC+1

```

```

      DO 90 I=IC1,MESH
      XJ(I)=0.0
90  RU(I)=RUFNL2(I)
91  CONTINUE
      DO 92 I=2,IC
92  RU(I)=RUFNL2(I)+XJ(I)*SNLG(I)
93  CCNTINUE
      IF (KUT) 94,96,94
94  ICUT=MESH
      LIMIT=MESH
      DO 95 I=2,MESH
      VLAST=V(I)
      V(I)=RU(I)/R(I)
95  XI(I)=V(I)-VLAST
      GO TO 102
96  CONTINUE
      ICUT=0
      DO 101 I=2,MESH
      VLAST=V(I)
      IF (ICUT) 97,97,99
97  IF (TWOZZZ+RU(I)) 100,100,98
98  ICUT=I
99  V(I)=TWOZZZ/R(I)
      GO TO 101
100 V(I)=RU(I)/R(I)
101 XI(I)=V(I)-VLAST
102 CONTINUE
      XI(1)=0.0

```

C
C
C

NEXT TRIAL EIGENVALUES PREDICTED BY PERTURBATION THEORY

```

      NCARDS=90
      DO 105 M=1,NCSPVS
      K=(NKKK(M)-1)/40
      H=0.0025*C
      ASUM=0.0
      A1=0.0
      I=1
      DO 104 J=1,K
      DO 103 L=1,40
      I=I+1
      A2=XI(I)*SNL(M,I)**2
103  A1=A1+A2*H
      ASUM=ASUM+A1*(A2/2.0)*H
      H=H+H
104  A1=(A2/2.0)*H
      EE(M)=EE(M)+ASUM
105  NCARDS=NCARDS+8*K+2
      GO TO 4E

```

C
C
C
C
C

WHEN NOCOPY=1 ALL RESULTS TRANS FROM INTERN MEMORY TO PRINT

WHEN NOCOPY=0 OUTPUT IS LAST ORBITAL WV. FNCT. ONLY

```

106 CONTINUE
      IF (NOCOPY) 107,114,107
107 CONTINUE
      PRINT 130, NCARDS,MCARDS
      NC=1

```

```

        WRITE (IM,135) Z,NCORE5,NVALES,ION,IZ,NC
        DO 110 I=1,441
          IF (TWOION+RUINL2(I)) 110,110,108
108    DO 109 M=1,441
109    RUINL2(M)=TWOION
        GO TO 111
110    CONTINUE
111    CONTINUE
        DO 112 MIN=1,440,5
          MAX=MIN+4
          NC=NC+1
          WRITE (IM,136) (RUINL2(M),M=MIN,MAX),IZ,NC
112    CONTINUE
          NC=NC+1
          WRITE (IM,137) RUINL2(441),IZ,NC
          DO 114 M=1,NCSPVS
            NLZ=NNLZ(M)
            KKK=NKKK(M)
            XL=NLZ/10=10*(NLZ/100)
            LP=XL+1.0
            NC=NC+1
            WRITE (IM,134) NLZ,XL,EE(M),WWNL(M),KKK,IZ,NC
            KI=KKK-1
            DO 113 MIN=1,KI,5
              NC=NC+1
              MAX=MIN+4
              WRITE (IM,136) (SNL(M,I),I=MIN,MAX),IZ,NC
113    CONTINUE
              NC=NC+1
              WRITE (IM,137) SNL(M,KKK),IZ,NC
114    CONTINUE
              IF (KEY=1) 115,116,118
115    KEY=1
116    DO 117 I=1,MESH
117    RU3(I)=RU(I)
          ZE3=Z
          GO TO 11
118    DO 119 I=1,MESH
          RU2(I)=RU3(I)
119    RU3(I)=RU(I)
          ZE2=ZE3
          ZE3=Z
          GO TO 11
120    CONTINUE

```

C
C
C

PUNCH GROUND STATE WAVE FUNCTIONS

```

        Z=AZ
        NC=0
        M=NCSPVS
        NLZ=NNLZ(M)
        KKK=NKKK(M)
        XL=NLZ/10=10*(NLZ/100)
        NC=NC+1
        WRITE (ID,142) NLZ,XL,EE(M),WWNL(M),KKK,Z,IZ,NC
        KI=KKK-1
        DO 121 MIN=1,KI,5
          NC=NC+1
          MAX=MIN+4

```

```

WRITE (ID,136) (SNL(M,I),I=MIN,MAX),IZ,NC
121 CONTINUE
NC=NC+1
WRITE (ID,137) SNL(M,KKK),IZ,NC
C
C CALCULATE EXCITED STATE WAVE FUNCTIONS
C
DO 123 KC=1,JE
M=NCSPVS+1
READ (IR,127)>NNLZ(M),WWNL(M),EE(M)
WWW=0.0
WWW=WWW+WWNL(M)
E=EE(M)
NN>NNLZ(M)/100
LAM>NNLZ(M)/10=10*NN
XL=LAM
CALL SCHEQ (Z,E,LAM,NN,KKK,MESH,C,THRESH)
C
C PUNCH EXCITED STATE WAVE FUNCTIONS
C
NC=0
M=NCSPVS+1
NLZ>NNLZ(M)
XL=NLZ/10=10*(NLZ/100)
NC=NC+1
WRITE (ID,142) NLZ,XL,EE(M),WWNL(M),KKK,Z,IZ,NC
K1=KKK-1
DO 122 MIN=1,K1,5
NC=NC+1
MAX=MIN+4
WRITE (ID,136) (SNLO(I),I=MIN,MAX),IZ,NC
122 CONTINUE
NC=NC+1
WRITE (ID,137) SNLO(KKK),IZ,NC
123 CONTINUE
CALL EXIT
C
124 FORMAT (F8.5,9F7.5)
125 FORMAT (F4.0,3I4)
126 FORMAT (6H WWW= F4.0,6H ZZZ= F4.0,6H Z= F4.0,10H NCDRES=I4,11H
1 NVALES= I4,11H NCSPVS= I4/25H CONTROL CARDS INCORRECT.)
127 FORMAT (I4,F4.0,C,F8.4)
128 FORMAT (I7,F7.0,C,1PE14.7,OP2(I6,F9.3))
129 FORMAT (1PE15.7,1P4E14.7)
130 FORMAT (10H NCARDS= I4,10H MCARDS=I4)
131 FORMAT (I4,2F8.6,11I4)
132 FORMAT (8H KEY = I4)
133 FORMAT (6H ITER,7X,1HZ,4X5HDELTA,7X,30HI(DEL) X(DEL) I(CUT) X(
1 CUT))
134 FORMAT (I4,1P3E14.7,I4,1PE14.7,8X,1HZ,I3,I4)
135 FORMAT (F4.0,3I4,56X,1HZ,I3,I4)
136 FORMAT (1PE15.7,1P4E14.7,1X,1HZ,I3,I4)
137 FORMAT (1PE15.7,57X,1HZ,I3,I4)
138 FORMAT (72H
1 )
139 FORMAT (27HSTARTING POTENTIALS AND Z=,F4.0,9H IN ERROR,2F4.0)
140 FORMAT (40HII,X,RU3,RUINL1,RUFNL1,RUINL2,RUFNL2,RU )
141 FORMAT (I8,F10.4,1P6E16.7)
142 FORMAT (I4,1P3E14.7,I4,OPF4.0,18X,1HZ,I3,I4)

```

END
SUBROUTINE SCHEQ (ZZ,EN,LAMBDA,NOFL,KKK,MESH,SCF,THRESH)

SUBROUTINE SCHEQ

COMPUTE ENERGY EIGENVALUE AND WAVE FUNCTION

ORIGINALLY WRITTEN BY SHERWOOD SKILLMAN

RCA LABORATORIES, PRINCETON, NEW JERSEY, SPRING 1961

MODIFIED BY FRANK HERMAN, SUMMER 1961

FURTHER MODIFIED BY RICHARD KORTUM AND PAUL KELLY, LOCKHEED
RESEARCH LABORATORIES, PALO ALTO, CALIFORNIA, SUMMER 1962

POTENTIAL AVAILABLE IN COMMON STORAGE AT START. WAVE FUNCTION,
COMPUTED EIGENVALUE, AND KKK LOCATED IN COMMON STORAGE AT
RETURN FROM SCHEQ.

NOTATION: ATOMIC NUMBER(ZZ=Z); TRIAL EIGENVALUE(EN=E); ORBIT.
QUANT. NO.(LAMBDA=XL); PRINC. QUANT. NO.(NOFL=N); NO. OF MESH
PTS. USED FOR WV. FNCT.(KKK); NO. OF INTEGRATION MESH PTS.
(MESS=MESH); SCALE FACTOR(SCF); EIGENVALUE ACCUR. CRIT.(THRESH)

DIMENSION P(5), Q(5), T(5), D(5)
DIMENSION R(521), RSCORE(521), RUINL1(521), RU2(521), RU(521),>NNL
1Z(24), RSVALE(521), RUFNL1(521), RU3(521), XI(521), WWNL(24), V(52
21), RSATOM(521), RUINL2(521), XNUM(521), XJ(521), NKKK(24), EE(24)
3, RUEXCH(521), RUFNL2(521), DENM(521), SNL(10,521), SNLO(521), QQ(
4521)

COMMON V,SNLO,R,RSCORE,RSVALE,RU,RUEXCH,XI,XJ,RSATOM,SNL,RUINL1,RU
1FNL1,RUINL2,RUFNL2,RU2,RU3,>NNLZ,WWNL,NKKK,EE
EQUIVALENCE (RSCORE,XNUM), (RSVALE,DENM), (QQ,RSATOM)

SET UP CONSTANTS AND INITIALIZE

IR=5
IP=6
IM=6
Z=ZZ
LAM=LAMBDA
NN=NOFL
MESH=MESH
C=SCF
MANY=200
E=EN
MOREV=0
LESSV=C
EMORE=0.0
ELESS=0.0
MORE=0
LESS=0
CE=0.0
NPRINT=0
LAMB=LAM-1
LAMP=LAM+1
XLP=LAMP
NCCR=NN-LAMP
B=LAM*LAMP
OC=R(2)
F=OC
FSQ=H*H
B3=(V(3)-V(2))/H=Z/HSQ


```

Y=H+H
FLPS=4*LAM+6
SLPT=6*LAM+12
ELPT=8*LAM+20
A1=Z/XLP
YSQ=Y*Y
B1=Z-Z
AB1=A1*B1
AB3=A1*B3
C
C
C
RAISE H AND Y TO LAM+1

HTL=H
YTL=Y
IF (LAM) 6,3,1
1 DO 2 I=1,LAM
  HTL=HTL*H
2 YTL=YTL*Y
3 H1=HSQ
  BCHS=B/HSQ
  EOH=B1/H
  PTH=B3*H
  EQ3=BOHS+BOH+BTH
  EQ4=BOHS/4.+BOH/2.+BTH+BTH
  EPL=8*LAM
  FPL=5*LAM
  XIFC=C*.21701389E-4
C
C
C
START OUTWARD INTEGRATION

4 NPRINT=NPRINT+1
  EPS=E-EG
  EG=E
  IF (MANY=NPRINT) 5,8,8
5 WRITE (IP,95) NN,LAM,Z
  CALL EXIT
6 NSTOP=77
7 WRITE (IP,96) NSTOP
  CALL EXIT
8 DO 9 I=1,MESH
9 SNLO(I)=C.0
  IF (NPRINT=1) 6,10,17
10 CONTINUE
  DO 11 I=4,MESH
    QQ(I)=V(I)+B/(R(I)*R(I))-E
11 CONTINUE
12 M=MESH
  DO 14 I=4,MESH
    IF (QQ(M)) 13,14,14
13 IK=M+1
  GO TO 15
14 M=M-1
  NSTOP=521
C
C
C
Q IS EVERYWHERE POSITIVE

GO TO 7
15 IF (MESH=IK) 16,16,19
16 EPS=QQ(MESH-40)

```

```

      E=E+EPS
17  CONTINUE
      DO 18 I=4,MESH
18  QQ(I)=QQ(I)-EPS
      GO TO 12
19  CONTINUE
      NCROSS=0
      SIGN=1.0
      H=OC
      Y=H+H
C    B= LAM*(LAM+1)
C    B1= -2.*Z
      B2=3.0*Z/H-E+2.0*V(2)-V(3)
C    B3=(V(3)-V(2))/H =Z/HSQ
C    A1= -Z/(LAM+1)
      A2=(AB1+B2)/FLPS
C    A2=(A1*B1+B2)/(4*LAM+6)
      A3=(A2*B1+A1*B2+B3)/SLPT
C    A3=(A2*B1+A1*B2+B3)/(6*LAM+12)
      A4=(A3*B1+A2*B2+AB3)/ELPT
C    A4=(A3*B1+A2*B2+A1*B3)/(8*LAM+20)
      P(3)=(1.0+H*(A1+H*(A2+H*(A3+H*A4))))*HTL
C    P(3)=(1.0+A1*H+A2*H**2+A3*H**3+A4*H**4)*H**(XL+1.0)
      P(4)=(1.0+C*Y*(A1+Y*(A2+Y*(A3+Y*A4))))*YTL
C    P(4)=(1.0+C*A1*Y+A2*Y**2+A3*Y**3+A4*Y**4)*Y**(XL+1.0)
      Q(3)=BQ3+B2
C    Q(3)=(B+B1*H+B2*H**2+B3*H**3)/H**2
      Q(4)=BQ4+B2
C    Q(4)=(B+B1*Y+B2*Y**2+B3*Y**3)/Y**2
      SNLO(2)=P(3)
      SNLO(3)=P(4)
      I=3
      DX=OC
      H1=H**2
      H2=H1/12.0
      T(3)=P(3)*(1.0-H2*Q(3))
      T(4)=P(4)*(1.0-H2*Q(4))
      C(4)=T(4)-T(3)
      NCOUNT=3
      NINT=2
20  I=I+1
C
C    IF END OF MESH IS REACHED, MODIFY TRIAL EIGENVALUE
C
      IF (I=MESH) 22,21,21
21  IF (NDCR=NCROSS) 37,44,44
C
C    RETURN TO BEGINNING OF OUTWARD INTEGRATION IF NECESSARY
C
22  Q(5)=QQ(I)
      IF (IK=I) 34,34,23
23  D(5)=D(4)+H1*Q(4)*P(4)
      T(5)=D(5)+T(4)
      IF (1.0=ABS(H2*Q(5))) 21,21,24
24  P(5)=T(5)/(1.0-H2*Q(5))
      SNLO(I)=P(5)
      IF (SIGN) 25,6,26
25  IF (P(5)) 28,28,27
26  IF (P(5)) 27,28,28

```

```

27 NCROSS=NCROSS+1
C
C   COUNT CHANGES IN SIGN
C
SIGN=-SIGN
28 NCOUNT=NCOUNT+1
   IF (7=NCOUNT) 6,29,30
29 NCOUNT=2
30 NINT=NINT+1
   IF (40=NINT) 6,31,32
31 DX=DX+DX
   H=DX
   H1=H**2
   H2=H1/12.0
   NINT=0
   T(5)=P(5)*(1.0-H2*Q(5))
   T(3)=P(3)*(1.0-H2*Q(3))
   C(5)=T(5)-T(3)
32 DO 33 K=1,4
   P(K)=P(K+1)
   T(K)=T(K+1)
   D(K)=D(K+1)
33 Q(K)=Q(K+1)
   GO TO 20
34 IF (NCOUNT=2) 6,35,23
35 IF (NINT=4) 23,23,36
C
C   MATCHING RADIUS HAS BEEN REACHED GOING OUT
C
C   IF NDCR NOT EQUAL TO NCROSS, MODIFY TRIAL EIGENVALUE
C
36 EIGEN=E
   IF (NDCR=NCROSS) 37,52,44
37 MORE=1
C
C   TOO MANY CROSSINGS, INCREASE ABSF(E)
C
MOREV=MOREV+1
   IF (MOREV=1) 38,40,35
38 NSTOP=50
   GO TO 7
39 IF (E=EMORE) 40,41,41
40 EMORE=E
41 IF (LESS) 42,43,51
42 NSTOP=55
   GO TO 7
43 E=1.25*EG
   GO TO 4
44 LESS=1
C
C   TOO FEW CROSSINGS, DECREASE ABSF(E)
C
LESSV=LESSV+1
   IF (LESSV=1) 45,47,46
45 NSTOP=57
   GO TO 7
46 IF (ELESS=E) 47,48,48
47 ELESS=E
48 IF (MORE) 49,50,51

```

```

49 NSTOP=62
   GO TO 7
50 E=0.75*EG
   GO TO 4
51 E=0.5*(EMORE+ELESS)
   GO TO 4
52 IF (ABS(SNLO(I=1))-ABS(SNLO(I=2))) 53,56,56
C
C   CHECK TO SEE THAT WAVE IS IN THE DAMPED REGION (ABSOLUTE VALUE
C   DECREASING AND SIGNS ALIKE)
C
53 IF (P(5)) 54,23,55
54 IF (SNLO(I=2)) 57,23,23
55 IF (SNLO(I=2)) 23,23,57
56 IF (1.0E+25=ABS(P(5))) 44,44,23
C
C   LARGE ABSOLUTE VALUE OF P IN WHAT SHOULD BE THE DAMPED REGION
C   INDICATES TOO FEW PEAKS, DECREASE ABSF(E)
C
C   NOW NDCR = NCROSS AND MATCHING RADIUS LIES IN DAMPED REGION
C
57 IMATCH=I-2
   XMATCH=R(I-2)
   PPOUT=(T(4)-T(2)-0.5*(P(4)-P(2)))/H
   S2=PPOUT/P(3)
C
C   INTEGRATION IS BY 8 APPLICATIONS OF NEWTON-COTES CLOSED
C   QUADRATURE FOR FIVE INTERVALS ON EACH BLOCK
C
C   XIFC =(5*H(BLOCK-1)/288)/2 ,H(1) =0.0025*SCALE FACTOR
C
   SUM1=0.0
   XIF=XIFC
   I=1
   VALUE=C.0
58 MM=8
   SUM2=0.0
   XIF=XIF+XIF
59 Y=VALUE
   VALUE=SNLO(I+5)**2
   SUM2=SUM2+19.0*(VALUE+Y)+75.0*(SNLO(I+4)**2+SNLO(I+1)**2)+50.0*(SN
   LO(I+2)**2+SNLO(I+3)**2)
   I=I+5
   IF (IMATCH=I) 6,62,60
60 MM=MM-1
   IF (MM) 6,61,59
61 SUM1=SUM2*XIF+SUM1
   GO TO 58
62 SUM1=SUM1+SUM2*XIF
   S1=SUM1/P(3)**2
   PMATCH=P(3)
   IF (NN=1) 6,63,64
63 XINW=EPL*XMATCH
C
C   FOR N =1, START INWARD INTEGRATION AT(8+LAM)*XMATCH OR X MAX
C
   GO TO 65
64 XINW=FPL*XMATCH
C

```

```

C      FOR N NOT=1, START AT (5+LAM)*XMATCH OR X MAX (END OF MESH)
C
65 DO 67, I=41, MESH, 40
   IF (XINH=R(I)) 66, 66, 67
66 KKK=I
   GO TO 68
67 CONTINUE
   KKK=MESH
68 I=KKK
   DX=R(I)-R(I-1)
   H=DX
   XIF=0.17361111E=1*DX
   HSQ=H*H
   HSQ12=HSQ/12.0
   Q(3)=QQ(I)
   P(3)=EXP(-R(I)*SQRT(Q(3)))
   SUM3=P(3)/Q(3)
   I=I-1
   Q(4)=QQ(I)
   P(4)=EXP(-R(I)*SQRT(Q(4)))
   IF (ABS(P(4))-1.0E=35) 69, 69, 71
69 KKK=KKK-40
   IF (KKK=IMATCH) 70, 70, 68
70 WRITE (IP, 97) Z, NN, LAM, KKK
   KKK=KKK+40
   P(4)=1.0E=35
   P(3)=1.0E=35
71 IF (PMATCH) 72, 6, 73
72 P(3)=P(3)
   P(4)=P(4)
73 SNLO(I+1)=P(3)
   SNLO(I)=P(4)
   T(3)=P(3)*(1.0=HSQ12*Q(3))
   T(4)=P(4)*(1.0=HSQ12*Q(4))
   C(4)=T(4)-T(3)
74 DO 76 M=2, 40
   I=I-1
   Q(5)=QQ(I)
   C(5)=HSQ*Q(4)*P(4)+D(4)
   T(5)=D(5)+T(4)
   P(5)=T(5)/(1.0=HSQ12*Q(5))
   IF (I=IMATCH+1) 6, 78, 75
75 SNLO(I)=P(5)
   DO 76 K=1, 4
   P(K)=P(K+1)
   T(K)=T(K+1)
   C(K)=D(K+1)
76 Q(K)=Q(K+1)
   Q(5)=QQ(I-2)
   C(5)=HSQ*Q(4)*P(4)+D(4)
   T(5)=D(5)+T(4)
   P(5)=T(5)/(1.0=HSQ12*Q(5))
   P(5)=1.09375*P(4)+0.2734375*P(5)=0.546875*P(3)+0.21875*P(2)=0.0390
1625*P(1)
   I=I-1
   CX=DX/2.0
   Q(5)=QQ(I)
   H=DX
   HSQ=H*H

```

```

HSQ12=HSQ/12.0
T(5)=P(5)*(1.0-HSQ12*Q(5))
T(4)=P(4)*(1.0-HSQ12*Q(4))
D(5)=T(5)-T(4)
SNLO(I)=P(5)
DO 77 L=1,4
P(L)=P(L+1)
T(L)=T(L+1)
D(L)=D(L+1)
77 Q(L)=Q(L+1)
GO TO 74

C
C   MATCHING RADIUS HAS BEEN REACHED COMING IN
C

78 K=KKK
VALUE=SNLO(K)**2
GO TO 80
79 CONTINUE
SUM3=SUM3+XIF*SUM4
XIF=XIF*C.5
80 MM=8
SUM4=0.0
81 Y=VALUE
VALUE=SNLO(K=5)**2
SUM4=SUM4+19.0*(VALUE+Y)+75.0*(SNLO(K=1)**2+SNLO(K=4)**2)+50.0*(SN
ILO(K=2)**2+SNLO(K=3)**2)
K=K+5
IF (K=IMATCH) 6,83,82
82 MM=MM+1
IF (MM) 6,79,81
83 SUM3=SUM3+XIF*SUM4
S3=SUM3/P(4)**2
PPIN=(T(5)-T(3)-C.5*(P(5)-P(3)))/H
S4=PPIN/P(4)
DE=(S2-S4)/(S1-S3)
IF (ABS(DE/E)=THRESH) 86,84,84
84 E=E+DE
IF (E) 4,85,85
85 E=E-DE
DE=DE/2.0
GO TO 84

C
C   IMPROVE TRIAL EIGENVALUE BY PERTURBATION THEORY IF NECESSARY
C   CALCULATE THE NORMALIZED WAVE FUNCTIONS
C

86 POP=PMATCH/P(4)
DO 87 J=IMATCH,KKK
87 SNLO(J)=SNLO(J)*POP
SUM1=0.0
J=1
XIF=XIFC
VALUE=0.0
88 MM=8
XIF=XIF+XIF
SUM2=0.0
89 Y=VALUE
VALUE=SNLO(J+5)**2
SUM2=SUM2+19.0*(VALUE+Y)+75.0*(SNLO(J+4)**2+SNLO(J+1)**2)+50.0*(SN
LO(J+2)**2+SNLO(J+3)**2)

```

```

J=J+5
MM=MM-1
IF (MM) 6,90,89
90 SUM1=SUM1+XIF*SUM2
IF (KKK=J) 6,91,88
91 C1=SQRT(SUM1)
IF (SNLO(3)) 92,6,93
92 C1=C1
93 DO 94 I=1,KKK
94 SNLO(I)=SNLO(I)/C1
EN=E
RETURN

```

C

```

95 FORMAT (20H NO CONVERGENCE ON,I4,I1,F4.0)
96 FORMAT (5HSTOP,I4,8HIN SCHEQ)
97 FORMAT (6HOAT Z=,F6.0,6H NL=,I3,I1,7H KKK=,I5,23H IS LESS THAN
1 IMATCH=,I5,43H INWARD INTEGRATION WILL BE TRIED AT KKK+40.)
END

```

b) Discussion

This program HFSWF, is a modification to the program written by Herman and Skillman (1963), H+S. The original work contains subroutines not presented here. However, the two principle components of H+S, the main program "Hartree-Fock-Slater Self-Consistent Atomic Field Program" and the principle subroutine "Schrödinger Equation Subroutine" (SCHEQ) are used. The text H+S, gives several hundred pages of discussion and tables concerning these calculations and should be consulted for further discussion. The material here will be an overview of the principle logic of the program as highlighted by the "comment" cards in the program listing.

This program computes numerical radial wave functions for the elements by solving the H-F-S equation

$$\left[\frac{d^2}{dr^2} - \frac{\lambda(\lambda+1)}{r^2} - V(r) - E_{nl} \right] P_{nl}(r) = 0 \quad (142)$$

for each orbital in a given configuration of an atom using the self-consistent field technique. A reading of the program listing will be useful for the discussion that follows.

Let us examine those sections of the program developed by H+S and separately consider the modifications made for use in this work.

i) Herman and Skillman Program

Initially let us note that in order to have a common mesh for all atoms in the periodic table the

parameter x , was used as the independent variable in place of r , the true radial distance. This parameter x is defined

$$x = \frac{r}{\mu} \quad \text{where} \quad \mu = \left(\frac{1}{2} \right) \left(\frac{3\pi}{4} \right)^{2/3} \left(\frac{1}{Z} \right)^{1/3}$$

References will be made to the "x-mesh" and "r-mesh" in the following discussion.

The program begins by reading a heading card and some control parameters (KEY, TOL, THRESH, etc.) that determine the form of the potential, define the self-consistency criteria, and provide other control information. The allowed values and meanings of these control parameters are reviewed in the "User-Manual" (Appendix VII). After constructing the "x-mesh" array some, or all, of the normalized potentials $RU(M)$ are read depending on the value of KEY.

The configuration information (Z , number of core orbitals (NCORES), etc.) is read and for each orbital the number of electrons (WWNL) and starting eigenvalue is read. If only some of the starting values of the potential have been read (KEY = 0) or if the potential is to be constructed from other potentials (KEY = 2), the calculation of the full 441 point normalized potential $RU(M)$ is carried out.

From the normalized potential $RU(M)$ the starting potential $V(M)$ to be used in the HFS equation is constructed in either the modified (KUT = 1) or un-modified (KUT = 0) form by use of the relations

$$V(M) = \text{Min} \left[\frac{RU(M)}{R(M)}, -\frac{2Z}{R(M)} \right] \quad \text{or} \quad V(M) = \frac{RU(M)}{R(M)} \quad (143)$$

where $R(M)$ is the true radial distance. After initializing some counting parameters, (e.g. MITER, number of iterations; LIMIT, mesh value M where

$RU(M) = -2Z$ the iteration is begun. If the test $(MAXIT - NITER)$ shows that the number of iterations has exceeded the chosen limit, $MAXIT$, an error message is printed and the program ends. If the test succeeds (i.e. $MAXIT < ITER$) the following occurs for the iteration.

For each orbital, the Schrödinger equation is solved using the constructed potential $V(M)$. By calling SCHEQ the electronic densities for each orbital ($RSCORE(M)$ and $RSVALE(M)$) and the total electronic density ($RSATOM(M) = RSCORE(M) + RSVALE(M)$) are calculated.

The atomic exchange potential ($RUEXCH(M)$), the total coulomb potential $XI(M)$ and the final potential $XJ(M)$ are calculated. Defining $DELTA$ as the maximum difference between the starting potential, $RU(M)$, and the potential calculated from this set of wave functions, $XJ(M)$, that is

$$DELTA = \max | XJ(M) - RU(M) | \quad (144)$$

a comparison with the required tolerance for self-consistency, TOL , is made. If $DELTA < TOL$, self-consistency has been reached and transfer to the output routine is made. Otherwise an improved starting potential $RU(M)$ is calculated and another iteration is begun.

The improved starting potential is calculated from the initial and final potentials by a simple arithmetic average

$$RU(M) = \frac{RUI(M) + XJ(M)}{2} \quad (145)$$

or by use of the Pratt improvement scheme,

$$RU(M) = 2 RUI(M) + (1 - \alpha) XJ(M) \quad (146)$$

where $0 \leq \alpha \leq 0.5$ below $M = LIMIT$, $\alpha = 0$ above limit.

(For more discussion of the Pratt improvement scheme see Herman and

Skillman (1963), Chapter 4 or Pratt (1952)).

New trial eigenvalues for each orbital are calculated using perturbation theory,

$$E = E + \langle M | H' | M \rangle \quad (147)$$

With the improved potential and the new eigenvalues the next iteration is begun.

The output routine is either all the radial wave functions and the self-consistent potential (NOCOPY=1) or just the last orbital (NOCOPY = 0) as punched cards.

ii) Modifications for This Calculation.

As discussed earlier we seek the appropriate radial wave functions that are consistent with our simplifying assumptions of the inert-core-active electron approximation used in developing the cross-section expressions used in this calculation.

Having achieved a self-consistent set of radial wave functions and a self-consistent potential we enforce our simplifying assumptions by solving for the excited state orbital in the given potential. This is done by reading the eigenvalue of the excited state and the number of electrons in the excited state and solving the wave equation in the ground-state self-consistent potential by calling SCHEQ.

The wave function achieved is punched as output.

Using the IBM 360/75 computer, the program HFSWF had a run time of 29 sec for the CESIUM 6s and 6p wave function calculation.

2. Excitation Cross-Section Program

This program, named EXCSCT, is a calculation of total electron atom excitation cross-sections for a range of incident electron energies using one of four possible approximations to the scattering amplitude. The program consists of a main routine and six subroutines.

a) Listing

```
PROGRAM EXCSCT(INPUT)
```

```
=====
*
*           * * *   EXCSCT   * * *
*
* A FORTRAN PROGRAM TO CALCULATE EXCITATION CROSS-
* SECTIONS FOR THE ELECTRON IMPACT EXCITATION OF ATOMS.
*
* ENERGY IS MEASURED IN UNITS OF THRESHOLD ENERGY, EPSIL
* EPSIL IS MEASURED IN UNITS OF TWICE THE RYDBERG.
*
* IPROX=THE APPROXIMATION USED. ALLOWED VALUES ARE:
* (1=BORN; 2=DCHKUR; 3=BETHE; 4=MODIFIED BETHE).
*
* N.B. *** MODIFIED BETHE (IPROX=4) MAY ONLY BE USED FOR*
* OPTICALLY ALLOWED TRANSITIONS***
=====
```

```
*****
*           PROGRAM           *
* AND SUBROUTINES BY        *
* TOM J GREENE              *
* UNIVERSITY OF TOLEDO      *
* 1970-1973                 *
*****
```

```
REAL*8 AQ,BO(4),BQ
DIMENSION ZN(25), SIG(25), FX(1001), XMSH(1001), SG(8), EPSL(4), N
IL1(4), NL2(4), SIGM(25,4)
COMMON PIN(521), PF(521), C, RANS, Y(521), KKK
EXTERNAL BJ, RN
DATA N, ZN(1), ZN(2), ZN(3), ZN(4), ZN(5), ZN(6), ZN(7), ZN(8), ZN(9)/20, 1.
120, 1.35, 1.50, 1.75, 2.00, 2.33, 2.67, 3.00, 3.57, ZN(10), ZN(11), ZN(12), ZN(
213), ZN(14), ZN(15), ZN(16), ZN(17), ZN(18), ZN(19), ZN(20)/4.00, 5.00, 6.0
30, 7.00, 8.00, 10.00, 12.00, 15.00, 18.00, 21.00, 24.00/
NCC=0
IP=6
IM=5
IR=5
```

```
READ CONTRL CARD; N=NO. OF VALUES OF INCIDENT ENERGY;
NTC=TYPE OF SERIES; NC=NO. OF SERIES; NOTP=OUTPUT OPTION;
A=ELEMENT NAME.
NTC: 1=SINGLE CASE; 2=MULTIPLE APPROX.; 3=MULTIPLE WV. FNCT.
NOTP: 1=PUNCHED CARD; 2=SINGLE LIST; 3=MULTIPLE LIST;
```

```
READ (IM, 46) N, NTC, NC, NOTP, AQ
```

```
READ ENERGY RANGE
```

```
ZN(N)=VALUES OF INCIDENT ENERGY IN THRESHOLD UNITS.
```

```
IF (N.NE.=1) GO TO 1
```

```
N=19
```

```
GO TO 2
```

```
1 READ (IR, 47) (ZN(I), I=1, N)
```

```
2 CONTINUE
```

```

C   READ INPUT WAVE FUNCTIONS
    READ (IR,48) NLZ1,XL1,EE1,WWNL1,KKK1,Z
    K11=KKK1-1
    DO 3 MIN=1,K11,5
    MAX=MIN+4
    READ (IR,49) (PIN(I),I=MIN,MAX)
3  CONTINUE
    READ (IR,50) PIN(KKK1)
4  READ (IR,48) NLZ2,XL2,EE2,WWNL2,KKK2,Z
    K21=KKK2-1
    DO 5 MIN=1,K21,5
    MAX=MIN+4
    READ (IR,49) (PF(I),I=MIN,MAX)
5  CONTINUE
    READ (IR,50) PF(KKK2)
    KKK=AMIN0(KKK1,KKK2)
    C=0.885341381/2**(.333333333)
    EPSIL=(ABS(EE2-EE1)/2.)
    N1=NLZ1/10
    N2=NLZ2/10

C   READ THE APPROXIMATION ,IPROX.
C   IPROX VALUES ARE: 1=BORN; 2=OCHKUR; 3=BETHE; 4=MODIFIED BETHE.
6  READ (IM,51) IPROX,BQ

C   TRANSFER TO THE APPROPRIATE APPROXIMATION.
    MWTC=2
    IF ((IPROX.EQ.1.OR.IPROX.EQ.2) MWTC=1
    GO TO (26,7), MWTC

C   BETHE APPROXIMATION.

C   FIND RDMO
7  CONTINUE
    XLAM=ABS(XL2-XL1)
    LAM=XLAM
    IF ((IPROX.EQ.4).AND.(LAM.NE.1)) GO TO 35

C   CALL RDINT (RN,LAM,1.0)

C   RDMO=(RANS**2)

C   FIND ANGFACT
    ANGFACT=(2.*XL2+1.)*((TJ(XL1,XL2,XLAM)*(2.**XLAM)*(FACT(XLAM)/F
12.*XLAM)))**2)/(2.*XLAM+1.)

C   FIND CUTOFF FOR BETHE

C   ZW=30.
    WMAX=SQRT(2.*ZW*EPSIL)*(1.+SQRT((ZW-1.)/ZW))
    WMIN=SQRT(2.*ZW*EPSIL)*(1.-SQRT((ZW-1.)/ZW))
    WKIN=2.*ZW*EPSIL
    LAMIN=LAM
    LAMAX=XL2+XL1
C   FIND SBRNW
    WSUM=0.0
    WANS=0.0
    DELW=(WMAX-WMIN)/100.
    W=WMIN-DELW

```

```

KW=1
DO 11 IW=1,101
W=W+DELW
FW=0.0
DO 8 I=LAMIN,LAMAX
WI=I
CALL RDINT (BJ,I,W)
FW=(FW+(2.*XL2+1.)*(2.*WI+1.)*((TJ(XL1,XL2,WI)*RANS)**2))/W**3
8 CONTINUE
KW=-KW
IF ((IW=1)*(IW=101)*KW) 9,11,10
9 WSUM=WSUM+2.*FW
10 WSUM=WSUM+FW
11 WSUM=WSUM+FW
WANS=WSUM*DELW/3.
SGBRN=8.*WANS/WKIN
C CORRECTION FOR DEL=LAM=0 IN BETHE APPROX.
IF (LAM.NE.0) GO TO 12
XLAM=2.
LAM=2
CALL RDINT (RN,LAM,I.0)
RDMO=(RANS**2)
ANGFCT=(2.*XL2+1.)*((TJ(XL1,XL2,XLAM)*(2.**XLAM)*(FACT(XLAM)/FACT(
12.*XLAM)))**2)/(2.*XLAM+1.)
C
12 WFF=8.*RDMO*ANGFCT/WKIN
IF (LAM.EQ.1) GO TO 13
XLAM2=2.*XLAM-2.
WKUT=(XLAM2*SGBRN/WFF+WMIN**XLAM2)**(1./XLAM2)
GO TO 14
13 WKUT=(EXP(SGBRN/WFF)*WMIN)
14 CONTINUE
C
C FIND ENFCT
DO 17 I=1,N
XMAX=WKUT
XMIN=SQRT(2.*ZN(I)*EPSIL)*(1.=SQRT((ZN(I)-1.)/ZN(I)))
ZKIN=2.*ZN(I)*EPSIL
IF (XLAM.EQ.1.) GO TO 15
XKINT=(XMAX**((2.*XLAM-2.))/(2.*XLAM-2.))-(XMIN**((2.*XLAM-2.))/(2.*X
15 LAM-2.))
GO TO 16
15 XKINT=ALOG(XMAX/XMIN)
16 ENFCT=(8.*XKINT)/ZKIN
C
17 SIG(I)=RDMO*ANGFCT*ENFCT
IF (IPROX.EQ.3) GO TO 36
C
C MODIFIED BETHE CALCULATION
C
DO 25 I=1,N
IF (ZN(I).LT.1.5) GO TO 23
ZKIN=2.*ZN(I)*EPSIL
SZ=(ZN(I)-1.)/ZN(I)
STUFF=RDMO*ANGFCT*4./((3.*ZKIN)
DO 20 LP1=1,8
LP=LP1-1
XLP=LP
IF (LP.EQ.0) GO TO 18

```

```

      ZETA=((XLP+1.)*(F(1,LP,SZ)**2)+XLP*(SZ**2)*(F(2,LP+1,SZ)**2))*(SZ*
1*(XLP+.5))/(2.*XLP+1.)
      REST=(2.*XLP+1.)*ZETA/(XLP*(XLP+1.))
      GO TO 19
18 REST=(SZ**1.5)*(F(2,1,SZ)**2)
19 SG(LP1)=STUFF*REST
C
C   FIND SGMXL
      SGMXL=(2.*XLP+1.)/ZKIN
C
C   FIND L=ZERO
      IF (SG(LP1).LT.(.5*SGMXL)) GO TO 21
20 CONTINUE
      WRITE (6,52)
21 CONTINUE
      LC=LP-1
      IF (LP.EQ.0) LO=0
      XLO=LO
C
C   FIND LO=TERM
      TRMLO=((XLO+1.)**2)/(2.*ZKIN)
C
C   FIND SUM=TERM
      TRMSM=0.0
      DO 22 LS=1,LP
22 TRMSM=TRMSM+SG(LS)
C
C   FIND MOD. BETHE C=SECTION
      GO TO 24
23 SIG(I)=0.0
      GO TO 25
24 SIG(I)=SIG(I)+TRMLO-TRMSM
25 CONTINUE
      GO TO 36
C
C   PORN + OCHKUR
C
26 CONTINUE
      XMN=SQRT(2.*ZN(N)*EPSIL)*(1.+SQRT((ZN(N)-1.)/ZN(N)))
      XMN=SQRT(2.*ZN(N)*EPSIL)*(1.-SQRT((ZN(N)-1.)/ZN(N)))
      DELX=(XMN-XMN)/1000.
      X=XMN-DELX
      DO 28 IX=1,1001
      X=X+DELX
      LAMIN=ABS(XL2-XL1)
      LAMAX=XL2+XL1
      DO 27 I=LAMIN,LAMAX
      XI=I
      FX(IX)=0.0
C
      CALL RINT (BJ,I,X)
C
      FX(IX)=(FX(IX)+(2.*XL2+1.)*(2.*XI+1.)*((TJ(XL1,XL2,XI)*RANS)**2))/
1IX**3
27 CONTINUE
      XMSH(IX)=X
28 CONTINUE
C
C   FIND K=LIMITS AND COMPUTE SIG

```



```

DO 34 I=1,N
XMAX=SQRT(2.*ZN(I)*EPSIL)*(1.+SQRT((ZN(I)-1.)/ZN(I)))
XMIN=SQRT(2.*ZN(I)*EPSIL)*(1.-SQRT((ZN(I)-1.)/ZN(I)))
ZKIN=2.*ZN(I)*EPSIL
DO 29 J=LAMIN,LAMAX
XJ=J
FXMAX=0.0
FXMIN=0.0
CALL RDINT (BJ,J,XMAX)
FXMAX=(FXMAX+(2.*XL2+1.)*(2.*XJ+1.)*((TJ(XL1,XL2,XJ)*RANS)**2))/XM
1AX**3
CALL RDINT (BJ,J,XMIN)
FXMIN=(FXMIN+(2.*XL2+1.)*(2.*XJ+1.)*((TJ(XL1,XL2,XJ)*RANS)**2))/XM
1IN**3
29 CONTINUE

C
C BEGIN K=INTEGRATION
XSUM=0.0
XANS=0.0
LP=(XMIN-XMNN)/DELX+1.
LQ=1001.-(XMXN-XMAX)/DELX
C TEST FOR NO. OF INTG. PTS. EVEN FOR SIMSON'S RULE INTG.
XLP=LP
XLQ=LQ
T1=(LP+LQ)/2
T2=(XLP+XLQ)/2.
IF (T1-T2.EQ.0.0) GO TO 30
LQ=LQ-1
C FIND CORRECTIN (C1) USING TRAPEZOID INTG. APPROX.
30 DILX1=XMIN-XMSH(LP)
C1=(FX(LP)+FXMIN)*DILX1/2.
X=XMSH(LP)-DELX
KX=1
DO 33 IX=LP,LQ
XIX=IX
X=X+DELX
A=(1.-(X**2/ZKIN)+(X**2/ZKIN)**2)
IF (IPROX.EQ.1.) A=1.0
DSIG=FX(IX)*A
KX=KX
IF ((IX-LP)*(IX-LQ)*KX) 31,33,32
31 XSUM=XSUM+2.*DSIG
32 XSUM=XSUM+DSIG
33 XSUM=XSUM+DSIG
XANS=XSUM*DELX/3.
DILX2=XMAX-X
C2=(FX(IX)+FXMAX)*DILX2/2.
XANSC=XANS+C1+C2
34 SIG(I)=(8.*XANSC)/ZKIN
GO TO 36

C
C OUTPUT ROUTINES
C
35 WRITE (6,53)
CALL EXIT
36 IF (NOTP=2) 37,39,41
C
C NOTP=1;PUNCHED CARDS
37 NCC=NCC+1

```

```

      CO 38 I=1,N
      WRITE (IP,54) ZN(I),SIG(I),BQ,Z,AQ,N1,N2,EPSIL
38  CONTINUE
      IF (NCC.EQ.NC) GO TO 45
      GO TO (45,6,4), NTC

```

C

C

```

      NOTP=2; SINGLE LIST
39  NCC=NCC+1
      WRITE (IP,60) AQ,BQ
      WRITE (IP,61)
      WRITE (IP,62)
      WRITE (IP,63)
      WRITE (IP,57) Z,EPSIL,N1,N2
      WRITE (IP,55)
      WRITE (IP,56)
      CO 40 I=1,N,3
      WRITE (IP,55)
      WRITE (IP,59)
      WRITE (IP,58) ZN(I),SIG(I),ZN(I+1),SIG(I+1),ZN(I+2),SIG(I+2)
      WRITE (IP,59)
      WRITE (IP,55)
40  CONTINUE
      IF (NCC.EQ.NC) GO TO 45
      GO TO (45,6,4), NTC

```

C

C

```

      NOTP=3; MULTIPLE LIST
41  NCC=NCC+1
      CO 42 I=1,N
42  SIGM(I,NCC)=SIG(I)
      EPSL(NCC)=EPSIL
      BO(NCC)=BQ
      NL1(NCC)=N1
      NL2(NCC)=N2
      IF (NCC.NE.NC) GO TO 44
      WRITE (IP,66) A,Z
      WRITE (IP,61)
      WRITE (IP,62)
      WRITE (IP,63)
      WRITE (IP,67)
      CO 43 I=1,N
      WRITE (IP,64) ZN(I),SIGM(I,1),SIGM(I,2),SIGM(I,3),SIGM(I,4)
43  CONTINUE
      WRITE (IP,69) BO(1),BO(2),BO(3),BO(4)
      WRITE (IP,68) NL1(1),NL2(1),NL1(2),NL2(2),NL1(3),NL2(3),NL1(4),NL2
1(4)
      WRITE (IP,65) EPSL(1),EPSL(2),EPSL(3),EPSL(4)
      GO TO 45
44  GO TO (45,6,4), NTC

```

C

```

45  CONTINUE
      STOP

```

C

```

46  FORMAT (4I3,A8)
47  FORMAT (12F6.2)
48  FORMAT (I4,1P3E14.7,I4,0PF4.0)
49  FORMAT (1PE15.7,1P4E14.7)
50  FORMAT (1PE15.7)
51  FORMAT (I3,A8)
52  FORMAT (2X,'**ERROR**LP1 HAS EXCEEDED VALUE OF 8 ')

```

```

53 FORMAT (1X, '***ERROR*** MOD. BETHE CAN ONLY BE USED FOR OPTICAL TRA
   POSITIONS')
54 FORMAT (1X, F8.3, 2X, E10.3, A8, '( ', F3.0, ') ', 2X, A8, '( ', I2, '= ', I2, ') ',
   1(EPSIL= ', E10.3, ') ')
55 FORMAT (1X, '*****')
   1('*****')
56 FORMAT (1X, 3(' ', 4X, 'N', 5X, '| ', 5X, 'SIG(N)', 4X, ' '), ' ')
57 FORMAT (3X, '(AT. NO.= ', F4.0, ') ', 13X, '(EPSIL= ', 1PE10.3, ') ', 10X, '(NL
   1=N', 'L', ': ', I2, '= ', I2, ') ')
58 FORMAT (1X, 3(' ', 0PF8.3, 2X, '| ', 3X, 1PE10.3, 2X, ' '), ' ')
59 FORMAT (1X, 3(' ', 10X, '| ', 15X, ' '), ' ')
60 FORMAT (32X, A8, '= ', A8, '//')
61 FORMAT (6X, 'CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2). ')
62 FORMAT (6X, 'INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (E
   1PSIL). ')
63 FORMAT (6X, 'EPSIL IS IN UNITS OF TWICE THE RYDBERG. ')
64 FORMAT (2X, F8.3, 4(6X, 1PE10.3) //)
65 FORMAT (3X, 'EPSIL', 2X, 4(6X, 1PE10.3) //)
66 FORMAT (32X, A8, 15X, '(AT.NO.= ', F3.0, ') //')
67 FORMAT (1X, 5X, 'N', 2X, 4(10X, 'SIG(N)') //)
68 FORMAT (3X, '(NL=N', 'L', ': ', 4(6X, '( ', I2, '= ', I2, ') ', 3X))
69 FORMAT (3X, 'APPROX.', 4(8X, A8))
   END
   SUBROUTINE R0INT (GRND, LAM, X)

```

C
C
C

DO INTEGRATION OVER WAVE FUNCTIONS

```

COMMON PIN(521), PF(521), C, RANS, Y(521), KKK
YSUM=0.0
YANS=0.0
DELY=0.0025
Y(1)=0.0
YMIN=0.0
YMAX=0.1
KY=1
L=1
JY=41
1 DO 10 IY=L, JY
   IF (IY=1) 2, 4, 2
2 IF (IY=L) 5, 3, 5
3 Y(L)=YMIN
   GO TO 6
4 SMTX=0.0
   GO TO 7
5 Y(IY)=Y(IY-1)*DELY
6 CONTINUE
   W=C*Y(IY)*X
   F=GRND(LAM, W)
   SMTX=PF(IY)*F*PIN(IY)
7 KY=KY
   IF ((IY=L)*(IY=JY)*KY) 8, 10, 9
8 YSUM=YSUM+2.*SMTX
9 YSUM=YSUM+SMTX
10 YSUM=YSUM+SMTX
   YANS=DELY*YSUM/3.+YANS
   DELY=DELY*DELY
   L=JY
   JY=JY+40
   YSUM=0.0

```

```

YMIN=YMAX
YMAX=YMAX+40.*DELY
KY=1
IF (JY=KKK=1) 1,11,11
11 RANS=YANS*C
RETURN
END
FUNCTION BJ (L,W)
SW=SIN(W)
CW=COS(W)
L1=L+1
GO TO (1,2,3,4,5,6,7,8), L1
1 BJ=SW/W
RETURN
2 BJ=SW/(W**2)=CW/W
RETURN
3 BJ=3.*SW/(W**3)=3.*CW/(W**2)=SW/W
RETURN
4 BJ=15.*SW/(W**4)=15.*CW/(W**3)=6.*SW/(W**2)+CW/W
RETURN
5 BJ=105.*SW/(W**5)=105.*CW/(W**4)=45.*SW/(W**3)+10.*CW/(W**2)+SW/W
RETURN
6 BJ=945.*SW/(W**6)=945.*CW/(W**5)=420.*SW/(W**4)+105.*CW/(W**3)+15.*
SW/(W**2)=CW/W
RETURN
7 BJ=12285.*SW/(W**7)=12285.*CW/(W**6)=7140.*SW/(W**5)+2140.*CW/(W**
4)+240.*SW/(W**3)=23.*CW/(W**2)=SW/W
RETURN
8 BJ=184275.*SW/(W**8)=184275.*CW/(W**7)=108045.*SW/(W**6)+4095.*CW/
W**5+4020.*SW/(W**4)=450.*CW/(W**3)=30.*SW/(W**2)=CW/W
RETURN
END
FUNCTION RN (L,W)
RN=W**L
RETURN
END
FUNCTION TJ (X1,X2,X3)
C CALCULATE 3=J SYMBOL
A=X1+X2+X3
AF=FACT(A)
B=X1+X3+X2
BF=FACT(B)
C=X2+X3+X1
CF=FACT(C)
D=X1+X2+X3+1.
DF=FACT(D)
E=(X1+X2+X3)/2.
EF=FACT(E)
E1=E+X1
E1F=FACT(E1)
E2=E+X2
E2F=FACT(E2)
E3=E+X3
E3F=FACT(E3)
TJ=(SQRT(AF*BF*CF/DF))*(EF/(E1F*E2F*E3F))
RETURN
END
FUNCTION FACT (A)
C CALCULATE FACTORIAL OF A NUMBER (A).

```

```

FACT=1.
IF (A.EQ.0.0) A=1.0
J=A
DO 1 I=1,J
  B=I
1 FACT=FACT*B
RETURN
END
FUNCTION F (M,N,Z)
DIMENSION AL(8,8)

```

C

```

AL(1,1)=1.
AL(1,2)=1.
AL(2,2)=1.
AL(1,3)=.5
AL(2,3)=1.
AL(3,3)=1.5
AL(1,4)=.5
AL(2,4)=.5
AL(3,4)=1.5
AL(4,4)=2.5
AL(1,5)=.625
AL(2,5)=.5
AL(3,5)=.75
AL(4,5)=2.5
AL(5,5)=4.375
AL(1,6)=.875
AL(2,6)=.625
AL(3,6)=.75
AL(4,6)=1.25
AL(5,6)=4.375
AL(6,6)=7.875
AL(1,7)=1.3125
AL(2,7)=.875
AL(3,7)=.9375
AL(4,7)=1.25
AL(5,7)=2.1875
AL(6,7)=7.875
AL(7,7)=14.4375
AL(1,8)=2.0625
AL(2,8)=1.3125
AL(3,8)=1.3125
AL(4,8)=1.5625
AL(5,8)=2.1875
AL(6,8)=3.9375
AL(7,8)=14.4375
AL(8,8)=26.8125

```

C

```

XN=N
A=XN/(2.**(XN-1.))

```

C

```

B=.5*A*LOG((1.+SQRT(Z))/(1.-SQRT(Z)))

```

C

C

```

FIND E,C+C

```

C

```

N1=N+1
GO TO (1,8), M

```

C

```

FIND E

```

```

1 CONTINUE

```

```

      IF (N=1) 2,2,3
2  E=0.
   GO TO 6
3  E=0.
   DO 5 IP1=3,N1
   S=0.
   IP1M2=IP1-2
   DO 4 IN1=1,IP1M2
   XIN1=IN1
4  S=S+(Z**((IN1-1)))/(2.*(XIN1-1.)+1.)
5  E=E+AL(N1=IP1+1,N1)*(Z**((-IP1+2))*S
C  FIND D
6  C=AL(N1,N1)
C  FIND C
   C=0.
   DO 7 IP1=1,N1
   XIP1=IP1
7  C=C+AL(N1=IP1+1,N1)*(Z**((1.5-XIP1)))
   GO TO 15
C
C
C  FIND E
8  CONTINUE
   IF (N=1) 9,10,10
9  E=0.
   GO TO 13
10 E=0.
   DO 12 IP1=2,N1
   S=0.
   IP1M1=IP1-1
   DO 11 IN1=1,IP1M1
   XIN1=IN1
11 S=S+(Z**((IN1-1)))/(2.*(XIN1-1.)+1.)
12 E=E+AL(IP1,N1)*(Z**((-IP1+1))*S
13 CONTINUE
C  FIND D
   D=0.
C  FIND C
   C=0.
   DO 14 IP1=1,N1
   XIP1=IP1
14 C=C+AL(IP1,N1)*(Z**((.5-XIP1)))
C
C
15 F=A*(B*C=D=E)
   RETURN
C
   ENC

```

b) Discussion

This program calculates electron impact excitation atomic cross-sections for a given range of incident energies using one of the following approximations to the scattering amplitude; Born, Bethe, Modified Bethe, or Ochkur.

The program begins by initializing the incident energy matrix $ZN(N)$ to a standard set of 20 values, and by assigning values to the read-write parameters IP, IM, IR. A control card is then read to control parameters whose meaning and allowed values are discussed in the User Manual--Appendix VII.

Depending on the value of N the incident energy values specified by the user are read in ($N \neq -1$), or the standard values are retained ($N = -1$). The initial and final state wave functions and related data (i.e. eigenenergies, EEl; orbital quantum number, XLI; etc.) are then read. The approximation to be used for this calculation is then read and the calculation begins.

Control is transferred to one of two major sections of the program depending on the approximation used. If the Born or Ochkur is used a "switch" parameter, MWTCH is set to 1 and the control moves to statement 26. Otherwise MWTCH is set to 2 and the program continues at statement 7. Statement 7 begins the Bethe, Modified Bethe section of the program. After testing to determine whether or not the Modified Bethe approximation is being used, the transition is checked to see if it is optically allowed ($\Delta l = 1$), then the radial integral

$$\int_0^{\infty} dr r^2 R_{n_i l_i}(r)^2 R_{n_f l_f}$$

is calculated by calling the subroutine RDINT. (If the Modified

Bethe optical allowed test fails an error message is printed and the program ends.) The angular factor ANGFACT is then calculated by calling the 3-j symbol subroutine TJ(XLI, XLZ, XLAM).

As is usually done in Bethe calculations the limits on the momentum transfer integral are cut-off by fitting the Bethe curve to a Born cross-section for a particular value of incident energy at high energy. This is done by using an incident energy value of 30 threshold units, and computing the Born cross-section for that value and finding a cut-off value for KMAX of WKUT. In the Bethe calculation, if the change in angular momentum, LAM is 0 the quadrupole moment is the first non-zero term in the Bethe series. The test is made and if necessary LAM is set equal to 2.

A particular value of the incident energy is next chosen and the energy term ENGFCT of the Bethe calculation is obtained.

The Bethe cross-section SIG(I) for the chosen energy value ZN(I) is calculated and the next energy value is chosen.

If the Bethe approximation is being used transfer to the output routine (statement 36) occurs after a cross-section for each energy has been computed. If the Modified Bethe approximation is being used, the additional terms for approximation are calculated as follows. An energy value is selected, ZN(1) a value of the final angular momentum LP is selected and the partial cross-section SG(LP1) is calculated. The "unitarity limit", Q_L^{\max} , cross-section for this value of LP is found and a test of Q_L is made. When the value of LP is

such that $Q_L < \frac{1}{2} Q_L^{\max}$ this value of LP is designated L0. The two correction terms for the Modified Bethe approximation TRML0, TRMSM are then found and subtracted from the Bethe Cross-section (as discussed in Chapter III). When this procedure is complete for all energy values transfer to the output routine (Statement 36) is made.

The next section of the program is for calculation of Born or Ochkur cross-sections.

For efficiency in the program the scattering amplitude $f_{\text{born}}(k)$ is found over the range KMAX(ZN(N)) to KMIN(ZN(N)) (where ZN(N) is the largest incident energy) and tabulated for 1000 values of f(k). The integration for the final cross-section for each energy value is then done by use of this table.

This section begins by calculating KMAX(ZN(N)) = XMXN and KMIN(ZN(N)) = XMNN. Then for a selected value within this range f(k) is found. This involves calling the radial integration sub-routine RDINT which includes the spherical Bessel function sub-routine BJ. When the table of values of f(k) (i.e. FX(IX)) is found, the calculation of the cross-sections for a particular value of the energy begins.

The limits on the K-integration (XMAX, XMIN) for the selected value of the energy ZN(I) are found. The value of the scattering amplitude at these limits FXMAX, FXMIN is found, and the integration over the range of K is begun. The closest value of XMAX, XMIN to the tabulated values are found, and those tabulated values are labeled LP and LQ respectively.

Since a Simpson's rule formula is used for the integration the number of integration points must be even. The value of LQ is adjusted to guarantee this and the integration $\int_{K(LO)}^{K(HQ)} \frac{d\sigma}{dk} dk$ is carried out using Simson's rule, and selecting either the Ochkur ($A \neq 1$) or Born ($A = 1$) expression.

The correction terms

$$\int_{K(LO)}^{K(HQ)} \frac{d\sigma}{dk} dk \quad \text{and} \quad \int_{K(LO)}^{K(HQ)} \frac{d\sigma}{dk} dk \quad \text{are}$$

found using a trapezoid integration and these correction terms are added to the tabular integration to obtain the cross-section SIG(I). Transfer to the output routine (Statement 36) is then made.

At Statement 36 control is transferred to one of the three output routines discussed in the user's manual.

When output has been completed, a test for the number of cases to be run is made and the program either ends or transfers back to read a new final state-wave function and approximation (Statement 4) or a new approximation (Statement 6).

Using the IBM 360/75 computer, the program EXCST for the CESIUM 6s-6p transition (where the radial entegral has 441 points) had the following run times:

Single Born case	=	2 min 3 sec
Single Ochkur case	=	2 min 2 sec
Single Bethe case	=	25 sec
Single Modified Bethe case	=	24 sec
4 approximations	=	4 min 18 sec

3. Ionization Cross-Section Program

This program, named IONCST, is a calculation of the ionization cross-section for a single value of Incident Electron Energy. The program consists of a main program and five subroutines.

a) Listing

```
PROGRAM IONCST(INPUT)
```

```
=====
*
*           * * *   IONCST   * * *
*
* A FORTRAN PROGRAM TO CALCULATE PARTIAL CROSS-SECTIONS
*   FOR NEUTRAL ATOMS IONIZED BY INCIDENT ELECTRONS
* THE CALCULATION USES NUMERICAL WAVE FUNCTIONS FOR THE
*   ATOM AND THE BORN-COULOMB APPROXIMATION
*
=====
```

```
*****
*           PROGRAM           *
*   AND SUBROUTINES BY      *
*   TOM J GREENE            *
*   UNIVERSITY OF TOLEDO    *
*           1973             *
*****
```

```
REAL*4 KAPA,KAPAMX
REAL*8 AQ
DIMENSION ZN(2), SGGL(6), ZL2(6)
EXTERNAL BJ,RN,FACT
COMMON PIN(521),PF(521),C,RANS,Y(521),KKK
ETAMAX=10.
ETAMIN=10.
RHOMAX=0.
RHOMIN=10.
IP=6
IM=5
IR=5
```

```
DO 15 ITG1=1,1
```

```
READ BOUND STATE WAVE FUNCTION
```

```
READ (IM,17) AQ
READ (IR,18) NLZ1,XL1,EE1,WWNL1,KKK1,Z
K11=KKK1-1
DO 1 MIN=1,K11,5
MAX=MIN+4
READ (IR,19) (PIN(I),I=MIN,MAX)
1 CONTINUE
READ (IR,20) PIN(KKK1)
EPSIL=(ABS(EE1)/2.)
PI=3.1415927
C=0.885341381/7**(.333333333)
KKK=KKK1
```

```
BOUND Y(11)
```

```
NBLOCK=KKK1/40
I1=1
Y(I1)=0.0
DELTAY=.0025
DO 3 J1=1,NBLOCK
DO 2 K1=1,40
```

```

      I1=I1+1
2  Y(I1)=Y(I1-1)+DELTAY
3  DELTAY=DELTAY+DELTAY
      PF(I1)=0.0

C
C  READ ENERGY IN THRESHOLD UNITS AND FIND X INITIAL
C
      N=1
      DO 15 I7G=1,1
      READ (IR,21) ZN(I1)
      XIN=SQRT(2.*EPSIL*ZN(I1))

C
      SG=0.0
C  PICK XL2 AND FIND LAMAX1 AND LAMIN1
      DO 14 IXL2P1=1,6
      IXL2=IXL2P1-1
      XL2=IXL2
      LAMIN1=ABS(XL2-XL1+1)
      LAMAX1=XL2+XL1+1

C
C  FIND KAPAMX AND PICK KAPPA
      DSGKAP=0.0
      KAPAMX=SQRT((ZN(I1)-1.)*EPSIL)
      SGLSUM=0.0
      DELKAP=KAPAMX/10.
      KAPA=0.0
      KS=1
      DSGL=0.0
      DO 13 IKS=1,11
      KAPA=KAPA+DELKAP
      ETA=1./KAPA
      ETAMAX=AMAX1(ETAMAX,ETA)
      ETAMIN=AMIN1(ETAMIN,ETA)
      TABULATE PF(EK,R,ETA,XL2)

C
C
      DO 4 I1=2,KKK1
      R=Y(I1)*C
      RHO=KAPA*R
      RHOMAX=AMAX1(RHOMAX,RHO)
      RHOMIN=AMIN1(RHOMIN,RHO)
      F=FLNR(IXL2,RHO,ETA)
      PF(I1)=FLNR(IXL2,RHO,ETA)*((2.*XL2+1.)/(KAPA*((2.*PI)**1.5)))
4  CONTINUE
      IF (XL1.NE.XL2) GO TO 6

C
C  ORTHOGONALIZE PF+PI (PF!=PF-C*PI)
C
      IJK=0
      XYZ=1.0
      CALL RDINT (RN,IJK,XYZ)
      CNR=RANS
      DO 5 I1=2,KKK
      PF(I1)=PF(I1)-CNR*PIN(I1)
5  CONTINUE
6  CONTINUE
C  FIND THE LIMITS ON THE K-INTEGRATION(200 PTS.)
C
      X=0.0

```

```

XFN=SQRT((=KAPA**2+2.*(ZN(1)=1.)*EPSIL)
XMIN=XIN-XFN
XMAX=XIN+XFN
DELX=(XMAX-XMIN)/20.
XSUM=0.0
XANS=0.0
X=XMIN-DELX
KX=1
DO 10 IX=1,21
X=X+DELX
FPR=0.0
FLAM=0.0
XINTG=0.0
DO 7 LAM1=LAMIN1,LAMAX1
LAM=LAM1-1
XLAM=LAM
CALL RDINT (BJ,LAM,X)
XTJ=TJ(XL1,XL2,XLAM)
7 FLAM=(2.*XLAM+1.)*((XTJ*RANS)**2)/(2.*XL2+1.)+FLAM
FPR=FLAM
XINTG=FPR/(X**3)
KX=KX
IF ((IX=1)*(IX=20)*KX) 8,10,9.
8 XSUM=XSUM+2.*XINTG
9 XSUM=XSUM+XINTG
10 XSUM=XSUM+XINTG
XANS=XSUM*DELX/3.
DSGL=(128.*XANS)*((KAPA*PI/XIN)**2)
KS=KS
IF ((KS=1)*(KS=11)*KS) 11,13,12
11 SGLSUM=SGLSUM+2.*DSGL
12 SGLSUM=SGLSUM+DSGL
13 SGLSUM=SGLSUM+DSGL
SGL=SGLSUM*DELKAP/3.
ZNLG=ALOG10(ZN(1))
N1=NLZ1/10
SGGL(IXL2P1)=SGL
ZL2(IXL2P1)=XL2
14 SG=SG+SGL
15 CONTINUE
C OUTPUT ROUTINE
WRITE (IP,22) AQ
WRITE (IP,27)
WRITE (IP,28)
WRITE (IP,29)
WRITE (IP,26) Z, EPSIL, N1
WRITE (IP,24)
WRITE (IP,25)
DO 16 I=1,6,3
WRITE (IP,24)
WRITE (IP,32)
WRITE (IP,31) ZL2(I), SGGL(I), ZL2(I+1), SGGL(I+1), ZL2(I+2), SGGL(I+2)
WRITE (IP,32)
16 CONTINUE
WRITE (IP,24)
WRITE (IP,23)
WRITE (IP,30) ZN(1), ZNLG, SG
WRITE (IP,23)
WRITE (IP,24)

```

```

WRITE (IP,34) RHOMAX,ETAMAX
WRITE (IP,33) RHOMIN,ETAMIN
WRITE (IP,24)
RETURN

```

C

```

17 FORMAT (A8)
18 FORMAT (I4,1P3E14.7,I4,OPF4.0)
19 FORMAT (IPE15.7,1P4E14.7)
20 FORMAT (IPE15.7)
21 FORMAT (I2F6.2)
22 FORMAT (32X,A8,'**COUL=BOHRN'//)
23 FORMAT (1X,'*',80X,'*')
24 FORMAT (1X,'*****')
1*****
25 FORMAT (1X,3('*',4X,'L',5X,'|',5X,'SIG(L)',4X),'*')
26 FORMAT (3X,'(AT. NO.=',F4.0,')',13X,'(EPSIL=',1PE10.3,'|',10X,'(NL
1=N',L',',12,'CONTINUUM)')
27 FORMAT (6X,'CROSS-SECTIONS ARE IN UNITS OF PI*(BOHR RADIUS**2).')
28 FORMAT (6X,'INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (E
1PSIL).')
29 FORMAT (6X,'EPSIL IS IN UNITS OF TWICE THE RYDBERG.'/)
30 FORMAT (1X,'*',8X,'N=',OPF8.3,8X,'LOG(N)=',1PE10.3,8X,'SIG(TOTAL)=
1',1PE10.3,16X,'*')
31 FORMAT (1X,3('*',OPF8.3,2X,'|',3X,1PE10.3,2X),'*')
32 FORMAT (1X,3('*',10X,'|',15X),'*')
33 FORMAT (1X,'*',RHO(MIN)=' ',1PE14.7,34X,ETA(MIN)=' ',1PE14.7,'*')
34 FORMAT (1X,'*',RHO(MAX)=' ',1PE14.7,34X,ETA(MAX)=' ',1PE14.7,'*')
END
FUNCTION FLNR (L,RHO,ETA)
XL=L
PI=3.14159265
FLNR=CLN*(RHO**(L+1))*PHI
C FIND CLN=PROD*(2.**L)*(SQRT(2.*PI*ETA))/(FACT(2.*XL+1.)*SQRT(1.=E
C (2.*PI*ETA))
C A=2.*PI*ETA
B=2.*XL+1.
C=ABS(1.-EXP(A))
FCT=FACT(B)
PROD=1.0
IF (L.EQ.0) GO TO 2
DO 1 I=1,L
S=I
PROD=PROD*SQRT(S**2+ETA**2)
1 CONTINUE
2 CONTINUE
CLN=PROD*(2.**L)*SQRT(-A)/(FCT*SQRT(C))
C FIND PHI=AKL*(RHO**K=L=1)
AKM2=1.0
AKM1=ETA/(XL+1.)
CSUM=1.0+AKM1*RHO
TCSUM=0.0
L3=L+3
L30=L+30
DO 3 K=L3,L30
XK=K
AK=(2.*ETA*AKM1-AKM2)/((XK+XL)*(XK-XL=1.))
IF ((RHO**(K=L=1)).LT.(1.E=40).AND.(AK.LT.1.E=20)) GO TO 4
CSUM=CSUM+AK*(RHO**(K=L=1))
TCSUM=CSUM

```

```

      AKM2=AKM1
      AKM1=AK
3    CONTINUE
4    CONTINUE
      PHI=CSUM
      FLNR=CLN*(RHO** (L+1))*PHI
      RETURN
      END
      SUBROUTINE RDINT (GRND,LAM,X)
C
C
C
      DO INTEGRATION OVER WAVE FUNCTIONS
      COMMON PIN(521),PF(521),C,RANS,Y(521),KKK
      YSUM=0.0
      YANS=0.0
      DELY=0.0025
      Y(1)=0.0
      YMIN=0.0
      YMAX=0.1
      KY=1
      L=1
      JY=41
1    GO TO (IY=L,JY
      IF ((IY=1) 2,4,2
2    IF ((IY=L) 5,3,5
3    Y(L)=YMIN
      GO TO 6
4    SMTX=0.0
      GO TO 7
5    Y(IY)=Y((IY=1)*DELY
6    CONTINUE
      W=C*Y(IY)*X
      F=GRND(LAM,W)
      SMTX=PF(IY)*F*PIN(IY)
      IP=6
7    KY=-KY
      IF (((IY=L)*(IY=JY)*KY) 8,10,9
8    YSUM=YSUM+2.*SMTX
9    YSUM=YSUM+SMTX
10   YSUM=YSUM+SMTX
      YANS=DELY*YSUM/3.+YANS
      DELY=DELY+DELY
      L=JY
      JY=JY+40
      YSUM=0.0
      YMIN=YMAX
      YMAX=YMAX+40.*DELY
      KY=1
      IF (JY=KKK=1) 1,11,11
11  RANS=YANS*C
      RETURN
      END
      FUNCTION BJ (L,W)
      IF (W.LT.1.) GO TO 8
      SW=SIN(W)
      CW=COS(W)
      LI=L+1
      GO TO (1,2,3,4,5,6,7), LI
1    BJ=SW/W

```



```

    RETURN
2  BJ=SW/(W**2)=CW/W
    RETURN
3  BJ=3.*SW/(W**3)=3.*CW/(W**2)=SW/W
    RETURN
4  BJ=15.*SW/(W**4)=15.*CW/(W**3)=6.*SW/(W**2)+CW/W
    RETURN
5  BJ=105.*SW/(W**5)=105.*CW/(W**4)=45.*SW/(W**3)+10.*CW/(W**2)+SW/W
    RETURN
6  BJ=945.*SW/(W**6)=945.*CW/(W**5)=420.*SW/(W**4)+105.*CW/(W**3)+15.
   1*SW/(W**2)=CW/W
    RETURN
7  BJ=10395.*SW/(W**7)=10395.*CW/(W**6)=4725.*SW/(W**5)+1260.*CW/(W**
   14)+210.*SW/(W**3)=21.*CW/(W**2)=SW/W
    RETURN
8  XL=L
   XN=XL+1.
   A=(W**2)/(2.*(2.*XL+3.))
   B=(W**4)/(8.*(2.*XL+3.)*(2.*XL+5.))
   BJ=((W**XL)*(2.**XN)*FACT(XN)/FACT(2.*XN))*(1.=A+B)
    RETURN
END
FUNCTION RN (L,W)
  RN=W**L
  RETURN
END
FUNCTION TJ (X1,X2,X3)
C  CALCULATE 3=J. SYMBOL
  A=X1+X2=X3
  AF=FACT(A)
  B=X1+X3=X2
  BF=FACT(B)
  C=X2+X3=X1
  CF=FACT(C)
  D=X1+X2+X3+1.
  DF=FACT(D)
  E=(X1+X2+X3)/2.
  EF=FACT(E)
  E1=E-X1
  E1F=FACT(E1)
  E2=E-X2
  E2F=FACT(E2)
  E3=E-X3
  E3F=FACT(E3)
  TJ=(SQRT(AF*BF*CF/DF))*(EF/(E1F*E2F*E3F))
  RETURN
END
FUNCTION FACT (A)
C  CALCULATE FACTORIAL OF A NUMBER (A).
  FACT=1.
  AA=A
  IF (A.EQ.0.0) AA=1.0
  J=AA
  DO 1 I=1,J
    B=I
    1 FACT=FACT*B
  RETURN
END

```

b) Discussion

This program calculates the first five partial-wave electron impact ionization cross-sections for a value of the incident energy using the Coulomb-Born approximation. The program consists of a main program and six subroutines.

It begins by reading the initial state radial wave function P_{IN} and related parameters (eigenenergy, orbital angular momentum, etc.) whose values are discussed in the User Manual--Appendix VII. After constructing the x-mesh (called $Y(I1)$) the incident energy is read.

The final state angular momentum quantum number (XLZ) is selected. For the particular value of the incident energy $ZN(I)$, the maximum allowed value of the wave vector for the secondary electron $KAPAMX$ is found. Within the range 0 to $KAPAMX$, a value of $KAPA$ is selected, and the integration over $KAPA$ is begun. For these values of XLZ and $KAPA$ the final state Coulomb wave function is found by calling the function $FLNR$.

If the initial orbital angular momentum XLI and the final angular momentum are the same the final state radial wave function is forced to be orthogonal to the initial state radial wave function, i.e. $PF = PF - [\int dr(PF)(P_{IN})] P_{IN} / N$.

The limits on the momentum transfer integral $XMAX$, $XMIN$, are found and the integral over the momentum transfer for this value of the secondary electron wave number is carried out. This is done by calling the radial integration routine $RDINT$, and by use of the 3-j symbol routine TJ .

Another value of the secondary electron wave number is selected and the process repeated until the maximum allowed value of $KAPAMX$ is reached, giving the partial cross-section Q_L for this value of the final angular momentum.

The next value of the final angular momentum is selected and the process is repeated until the Partial Cross-Section $Q(L)$ for $L = 0, 5$ are found. These partial cross-sections are added together to give the "total" ionization cross-section, SG , for this value of the incident energy.

The partial cross-section and the total cross-section are then printed out in the form shown in the User Manual.

Using the IBM 360/75 computer, the program IONCST had a run time of (7 min 6 sec) for the Helium case for one value of the incident energy. In this case the additional time is primarily due to the evaluation of the Coulomb wave function.

VI. SOME SAMPLE RESULTS FOR EXCITATION

In this chapter some results of the excitation cross-section calculations will be presented. Recall (Page 3) that for assessing the accuracy of various calculations the only methods available are those of comparing the cross-sections obtained in the various calculations with one another and with the limited experimental data available.

The tables presented will include reference data from other calculations and experimental work so that a comparison can be made. The two families of elements selected for presentation here were chosen to demonstrate what I expect to be the best and worst cases for the calculation. The Alkali family, which is an excellent approximation to the one-electron model, and the Inert family, where the inert-core-active electron assumption is weakest.

1) Tables

The two sets of tables will now be presented and a discussion of the results will follow.

a) Alkali Excitation Tables.

To establish a straight-forward comparison of the results of this calculation with the literature I chose to calculate cross-sections for the Alkali elements using the energy values of Vainshtein (1964). Vainshtein and his co-workers carried out a study of the Alkali family using the Born approximation that was reprinted in the classic work of Moiseiwitsch and Smith (1968). The organization of the Vainshtein tables has been used here. First the resonance (ns-np) transitions of the Alkalies are examined.

Then for each of the elements of the Alkali family, the first few transitions are calculated.

The Vainshtein* values are designated Born (1) in the tables that follow. The Born calculation of the present work is designated Born (2).

The energy range N is given in threshold units; the transition energy $EPSIL$ is in units of twice the Rydberg; and the cross-sections are measured in units of πa_B^2 .

*Vainshtein, L. A., V. Opykhtin, and L. Presnyakov, 1964a, P. N. Lebedev Institute of Physics Report A-53.

and

Vainshtein, L. A., V. Opykhtin, and L. Presnyakov 1964b, Zh. Eksperim. Teor. Fiz 47, 2306 English Transla: Soviet Physics. - JETP 18, 1383 (1964) as reprinted in Moiseiwitsch and Smith (1968).

ALKALI ELEMENT C-SECTION TABLES

Li:	2s-2p	Born(1),	Born(2),	Ochkur,	Bethe,	Mod. Bethe
Na:	3s-3p	Born(1),	Born(2),	Ochkur,	Bethe,	Mod. Bethe*
K:	4s-4p	Born(1),	Born(2),	Ochkur,	Bethe,	Mod. Bethe
Rb:	5s-5p	Born(1),	Born(2),	Ochkur,	Bethe,	Mod. Bethe
Cs:	6s-6p	Born(1),	Born(2),	Ochkur,	Bethe,	Mod. Bethe

Li:	2s-3p	Born(1),	Born(2),	Bethe,	Ochkur
	2s-4p	Born(1),	Born(2),	Bethe,	Ochkur
	2s-5p	Born(1),	Born(2),	Bethe,	Ochkur
	2s-3s	Born(1),	Born(2),	Bethe,	Ochkur
	2s-4s	Born(1),	Born(2),	Bethe,	Ochkur
	2s-5s	Born(1),	Born(2),	Bethe,	Ochkur
	2s-3d	Born(1),	Born(2),	Bethe,	Ochkur
	2s-4d	Born(1),	Born(2),	Bethe,	Ochkur
	2s-5d	Born(1),	Born(2),	Bethe,	Ochkur

For the remaining transitions Born(1), Bethe, and Ochkur results are given:

Na:	3s-4p	3s-4s	3s-3d	3s-7d
	3s-5p	3s-5s	3s-4d	
	3s-6p	3s-6s	3s-5d	
	3s-7p	3s-7s	3s-6d	
K:	4s-5p	4s-5s	4s-3d	4s-6d
	4s-6p	4s-6s	4s-4d	
	4s-7p	4s-7s	4s-5d	
Rb:	5s-6p	5s-6s	5s-4d	5s-7d
	5s-7p	5s-7s	5s-5d	
	5s-8p	5s-8s	5s-6d	
Cs:	6s-7p	6s-7s	6s-5d	6s-8d
	6s-8p	6s-8s	6s-6d	
	6s-9p	6s-9s	6s-7d	

Note (1): The use of the cut-off parameter in the Bethe calculation can lead to negative cross-section when $K_{\max} < K_{\min}$ for low values of the incident energy. These non-physical values have been set equal to zero.

*Note (2): Since the well-known sodium 3s-3p transition was recently the subject of a careful experimental study, the data from that study is given.

LITHIUM

2s-2p

EPSIL = 6.79 (-2)

SODIUM

3s-3p

EPSIL = 7.73 (-2)

N	BORN(1)	BORN(2)	OCHKUR	BETHE	MODBETHE	BORN(1)	BORN(2)	OCHKUR	BETHE	MODBETHE	EXP*
1.02	4.14(1)	4.07(1)	3.99(1)	6.96(0)	0.0	3.07(1)	3.08(1)	3.00(1)	0.0	0.0	1.75(1)
1.04	5.71(1)	5.62(1)	5.54(1)	2.43(1)	0.0	4.26(1)	4.27(1)	4.14(1)	0.0	0.0	1.81(1)
1.08	7.71(1)	7.58(1)	7.55(1)	4.68(1)	0.0	5.78(1)	5.79(1)	5.62(1)	0.0	0.0	1.94(1)
1.16	9.98(1)	9.81(1)	9.55(1)	7.36(1)	0.0	7.56(1)	7.58(1)	7.07(1)	2.50(1)	0.0	2.20(1)
1.32	1.20(2)	1.18(2)	1.14(2)	1.00(2)	0.0	9.32(1)	9.32(1)	8.45(1)	5.87(1)	0.0	2.72(1)
1.64	1.31(2)	1.28(2)	1.19(2)	1.18(2)	5.55(1)	1.04(2)	1.04(2)	9.14(1)	8.56(1)	1.80(1)	3.30(1)
2.28	1.24(2)	1.22(2)	1.10(2)	1.18(2)	6.38(1)	1.02(2)	1.03(2)	9.04(1)	9.56(1)	3.76(1)	3.52(1)
3.56	1.03(2)	1.01(2)	9.17(1)	9.98(1)	6.14(1)	8.84(1)	8.85(1)	8.07(1)	8.66(1)	4.43(1)	3.65(1)
6.12	7.53(1)	7.35(1)	6.92(1)	7.38(1)	5.06(1)	6.66(1)	6.66(1)	6.33(1)	6.67(1)	4.11(1)	3.56(1)
11.24	5.01(1)	4.89(1)	4.74(1)	4.93(1)	3.66(1)	4.54(1)	4.53(1)	4.42(1)	4.57(1)	3.17(1)	3.15(1)
21.48	3.12(1)	3.04(1)	3.00(1)	3.07(1)	2.40(1)	2.87(1)	2.87(1)	2.84(1)	2.90(1)	2.17(1)	2.42(1)
41.96	1.86(1)	1.81(1)	1.80(1)	1.83(1)	1.48(1)	1.73(1)	1.73(1)	1.72(1)	1.75(1)	1.37(1)	1.66(1)

* Linear Interpolation From "Enemark, E. A., and A. Gallagher, (1972) Phys. Rev. A, 6, 192".

POTASSIUM

4s-4p

EPSIL = 5.93 (-2)

RUBIDIUM

5s-5p

EPSIL = 5.78 (-2)

N	BORN(1)	BORN(2)	OCHKUR	BETHE	MODBETHE	BORN(1)	BORN(2)	OCHKUR	BETHE	MODBETHE
1.02	5.47(1)	5.51(1)	5.36(1)	0.0	0.0	5.85(1)	5.66(1)	5.47(1)	0.0	0.0
1.04	7.57(1)	7.65(1)	7.39(1)	0.0	0.0	8.11(1)	7.86(1)	7.54(1)	0.0	0.0
1.08	1.03(2)	1.04(2)	1.00(2)	0.0	0.0	1.10(2)	1.07(2)	1.02(2)	0.0	0.0
1.16	1.35(2)	1.37(2)	1.26(2)	2.77(1)	0.0	1.46(2)	1.42(2)	1.29(2)	1.11(0)	0.0
1.32	1.66(2)	1.69(2)	1.51(2)	9.58(1)	0.0	1.80(2)	1.78(2)	1.55(2)	8.33(1)	0.0
1.64	1.87(2)	1.91(2)	1.65(2)	1.52(2)	8.85(0)	2.03(2)	2.04(2)	1.73(2)	1.53(2)	0.0
2.28	1.86(2)	1.91(2)	1.67(2)	1.75(2)	4.80(1)	2.02(2)	2.07(2)	1.80(2)	1.86(2)	3.59(1)
3.56	1.59(2)	1.66(2)	1.51(2)	1.62(2)	6.92(1)	1.76(2)	1.82(2)	1.66(2)	1.76(2)	6.59(1)
6.12	1.20(2)	1.26(2)	1.20(2)	1.26(2)	6.86(1)	1.33(2)	1.39(2)	1.33(2)	1.39(2)	7.10(1)
11.24	8.21(1)	8.60(1)	8.41(1)	8.67(1)	5.54(1)	9.13(1)	9.60(1)	9.39(1)	9.67(1)	5.94(1)
21.48	5.20(1)	5.47(1)	5.41(1)	5.52(1)	3.89(1)	5.80(1)	6.13(1)	6.07(1)	6.19(1)	4.25(1)
41.96	3.14(1)	3.31(1)	3.29(1)	3.34(1)	2.51(1)	3.51(1)	3.72(1)	3.71(1)	3.76(1)	2.77(1)

CESIUM

6s-6p

EPSIL = 5.21 (-2)

N	BORN(1)	BORN(2)	OCHKUR	BETHE	MODBETHE
1.02	7.50(1)	7.06(1)	6.81(1)	0.0	0.0
1.04	1.04(2)	9.82(1)	9.38(1)	0.0	0.0
1.08	1.41(2)	1.35(2)	1.27(2)	0.0	0.0
1.16	1.86(2)	1.79(2)	1.60(2)	0.0	0.0
1.32	2.30(2)	2.26(2)	1.95(2)	8.78(1)	0.0
1.64	2.60(2)	2.62(2)	2.21(2)	1.88(2)	0.0
2.28	2.60(2)	2.69(2)	2.34(2)	2.39(2)	2.63(1)
3.56	2.26(2)	2.39(2)	2.19(2)	2.31(2)	7.27(1)
6.12	1.72(2)	1.85(2)	1.77(2)	1.84(2)	8.56(1)
11.24	1.17(2)	1.28(2)	1.25(2)	1.29(2)	7.45(1)
21.48	7.46(1)	8.21(1)	8.14(1)	8.29(1)	5.46(1)
41.96	4.52(1)	5.00(1)	4.98(1)	5.05(1)	3.61(1)

LITHIUM

2s-3p

EPSIL = 1.41 (-1)

N	BORN(1)	BORN(2)	BETHE	OCHKUR
1.02	9.67(-1)	9.74(-1)	2.76(-0)	9.72(-1)
1.04	1.30(0)	1.32(0)	2.72(-0)	1.34(-1)
1.08	1.68(0)	1.70(0)	2.64(-0)	1.79(-0)
1.16	2.01(0)	2.03(0)	2.48(-0)	2.15(-0)
1.32	2.11(0)	2.15(0)	2.21(-0)	2.29(-0)
1.64	1.87(0)	1.92(0)	1.80(-0)	1.90(-0)
2.28	1.39(0)	1.43(0)	1.33(-0)	1.27(-0)
3.56	8.91(-1)	9.22(-1)	8.71(-1)	7.34(-1)
6.12	5.20(-1)	5.37(-1)	5.19(-1)	4.66(-1)
11.24	2.88(-1)	2.94(-1)	2.90(-1)	2.69(-1)
21.48	1.55(-1)	1.56(-1)	1.56(-1)	1.49(-1)
41.96	8.23(-2)	8.16(-1)	8.19(-2)	7.95(-2)

2s-4p

EPSIL = 1.66 (-1)

BORN(1)	BORN(2)	BETHE	OCHKUR
2.24(-1)	2.27(-1)	3.24(-1)	2.28(-1)
3.01(-1)	3.05(-1)	3.30(-1)	3.14(-1)
3.84(-1)	3.90(-1)	3.35(-1)	4.16(-1)
4.49(-1)	4.56(-1)	3.33(-1)	4.95(-1)
4.67(-1)	4.67(-1)	3.18(-1)	5.10(-1)
3.91(-1)	4.02(-1)	2.82(-1)	4.04(-1)
2.84(-1)	2.93(-1)	2.26(-1)	2.56(-1)
1.84(-1)	1.89(-1)	1.62(-1)	1.56(-1)
1.13(-1)	1.13(-1)	1.05(-1)	9.76(-2)
6.67(-2)	6.55(-2)	6.39(-1)	5.99(-2)
3.85(-2)	3.69(-2)	3.69(-2)	3.53(-2)
2.19(-2)	2.05(-2)	2.07(-2)	2.00(-2)

LITHIUM

2s-5p

EPSIL = 1.78 (-1)

N	BORN(1)	BORN(2)	BETHE	OCHKUR
1.02	8.95(-2)	9.07(-2)	7.90(-2)	9.12(-2)
1.04	1.20(-1)	1.21(-1)	8.43(-2)	1.26(-1)
1.08	1.52(-1)	1.54(-1)	9.03(-2)	1.66(-1)
1.16	1.76(-1)	1.79(-1)	9.58(-2)	1.97(-1)
1.32	1.77(-1)	1.82(-1)	9.81(-2)	2.00(-1)
1.64	1.50(-1)	1.55(-1)	9.35(-2)	1.56(-1)
2.28	1.09(-1)	1.12(-1)	8.00(-2)	9.78(-2)
3.56	7.21(-2)	7.32(-2)	6.09(-2)	6.02(-2)
6.12	4.54(-2)	4.51(-2)	4.15(-2)	3.89(-2)
11.24	2.78(-2)	2.69(-2)	2.62(-2)	2.47(-2)
21.48	1.65(-2)	1.56(-2)	1.56(-2)	1.50(-2)
41.96	9.63(-3)	8.89(-3)	8.99(-3)	8.71(-3)

2s-3s

EPSIL = 1.24 (-1)

BORN(1)	BORN(2)	BETHE	OCHKUR
1.21(0)	1.23(-0)	1.03(0)	1.20(-0)
1.66(0)	1.68(-0)	1.83(0)	1.64(-0)
2.21(0)	2.24(-0)	2.72(0)	2.17(-0)
2.79(0)	2.83(-0)	3.55(0)	2.62(-0)
3.25(0)	3.27(-0)	4.04(0)	2.91(-0)
3.33(0)	3.32(-0)	3.94(0)	2.83(-0)
2.90(0)	2.88(-0)	3.23(0)	2.45(-0)
2.12(0)	2.10(-0)	2.25(0)	1.86(-0)
1.34(0)	1.33(-0)	1.37(0)	1.23(-0)
7.68(0)	7.55(-1)	7.66(-1)	7.24(-1)
4.12(0)	4.05(-1)	4.06(-1)	3.96(-1)
2.14(0)	2.10(-1)	2.10(-1)	2.08(-1)

LITHIUM

2s-4s

EPSIL = 1.60(-1)

N	BORN(1)	BORN(2)	BETHE	OCHKUR
1.02	2.13(-1)	2.17(-1)	4.43(-1)	2.11(-1)
1.04	2.91(-1)	2.96(-1)	5.31(-1)	2.86(-1)
1.08	3.86(-1)	3.91(-1)	6.24(-1)	3.76(-1)
1.16	4.84(-1)	4.88(-1)	7.00(-1)	4.47(-1)
1.32	5.55(-1)	5.56(-1)	7.24(-1)	4.86(-1)
1.64	5.58(-1)	5.56(-1)	6.64(-1)	4.64(-1)
2.28	4.76(-1)	4.71(-1)	5.25(-1)	3.96(-1)
3.56	3.42(-1)	3.37(-1)	3.57(-1)	2.97(-1)
6.12	2.13(-1)	2.09(-1)	2.15(-1)	1.93(-1)
11.24	1.20(-1)	1.18(-1)	1.19(-1)	1.13(-1)
21.48	6.43(-2)	6.30(-2)	6.31(-2)	6.15(-2)
41.96	3.32(-2)	3.25(-2)	3.25(-2)	3.22(-2)

2s-5s

EPSIL = 1.75 (-1)

BORN(1)	BORN(2)	BETHE	OCHKUR
7.81(-2)	7.89(-2)	1.83(-1)	7.65(-2)
1.07(-1)	1.08(-1)	2.10(-1)	1.04(-1)
1.41(-1)	1.42(-1)	2.36(-1)	1.36(-1)
1.76(-1)	1.76(-1)	2.59(-1)	1.60(-1)
2.01(-1)	2.00(-1)	2.62(-1)	1.73(-1)
2.00(-1)	1.98(-1)	2.37(-1)	1.65(-1)
1.60(-1)	1.67(-1)	1.85(-1)	1.40(-1)
1.21(-1)	1.18(-1)	1.25(-1)	1.04(-1)
7.50(-2)	7.32(-2)	7.52(-2)	6.76(-2)
4.23(-2)	4.12(-2)	4.17(-2)	3.94(-2)
2.25(-2)	2.19(-2)	2.20(-2)	2.14(-2)
1.16(-2)	1.13(-2)	1.13(-2)	1.12(-2)

LITHIUM

2s-3d

EPSIL = 1.43 (-1)

N	BORN(1)	BORN(2)	BETHE	OCHKUR
1.02	1.38(0)	1.31(-0)	0.0	1.26(-0)
1.04	1.90(0)	1.80(-0)	0.0	1.73(-0)
1.08	2.56(0)	2.43(-0)	0.0	2.31(-0)
1.16	3.31(0)	3.13(-0)	0.0	2.83(-0)
1.32	3.96(0)	3.73(-0)	9.82(-1)	3.24(-0)
1.64	4.19(0)	3.94(-0)	2.81(-1)	3.32(-0)
2.28	3.77(0)	3.52(-0)	3.18(-0)	3.01(-0)
3.56	2.82(0)	2.63(-0)	2.56(-0)	2.35(-0)
6.12	1.81(0)	1.69(-0)	1.67(-0)	1.58(-0)
11.24	1.04(0)	9.70(-1)	9.69(-1)	9.35(-1)
21.48	5.62(-1)	5.23(-1)	5.23(-1)	5.13(-1)
41.96	2.92(-1)	2.72(-1)	2.72(-1)	2.69(-1)

2s-4d

EPSIL = 1.67 (-1)

BORN(1)	BORN(2)	BETHE	OCHKUR
4.09(-1)	3.91(-1)	0.0	3.79(-1)
5.62(-1)	5.36(-1)	0.0	5.16(-1)
7.56(-1)	7.15(-1)	0.0	6.83(-1)
9.53(-1)	9.07(-1)	2.60(-1)	8.25(-1)
1.11(0)	1.06(-0)	7.26(-1)	9.22(-1)
1.14(0)	1.08(-0)	9.54(-1)	9.10(-1)
9.86(-1)	9.35(-1)	9.00(-1)	7.94(-1)
7.16(-1)	6.79(-1)	6.72(-1)	6.02(-1)
4.50(-1)	4.26(-1)	4.25(-1)	3.96(-1)
2.56(-1)	2.42(-1)	2.42(-1)	2.32(-1)
1.37(-1)	1.30(-1)	1.30(-1)	1.26(-1)
7.08(-2)	6.71(-2)	6.71(-2)	6.63(-2)

LITHIUM

2s-5d

EPSIL = 1.78 (-1)

N	BORN(1)	BORN(2)	BETHE	OCHKUR
1.02	1.79(-1)	1.71(-1)	0.0	1.66(-1)
1.04	2.45(-1)	2.35(-1)	0.0	2.26(-1)
1.08	3.26(-1)	3.12(-1)	2.23(-2)	2.98(-1)
1.16	4.10(-1)	3.93(-1)	2.14(-1)	3.58(-1)
1.32	4.73(-1)	4.52(-1)	3.65(-1)	3.95(-1)
1.64	4.78(-1)	4.57(-1)	4.25(-1)	3.84(-1)
2.28	4.08(-1)	3.90(-1)	3.82(-1)	3.30(-1)
3.56	2.93(-1)	2.80(-1)	2.78(-1)	2.47(-1)
6.12	1.82(-1)	1.74(-1)	1.74(-1)	1.61(-1)
11.24	1.03(-1)	9.85(-2)	9.85(-2)	9.43(-2)
21.48	5.50(-2)	5.26(-2)	5.26(-2)	5.14(-2)
41.96	2.85(-2)	2.72(-2)	2.72(-2)	2.69(-2)

SODIUM

3s-4p

3s-5p

3s-6p

EPSIL = 1.38 (-1)

EPSIL = 1.60 (-1)

EPSIL = 1.70 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	1.43(0)	6.61(-0)	1.40(-1)	3.85(-1)	1.66(-0)	3.75(-1)	1.64(-1)	6.77(-1)	1.59(-1)
1.04	1.95(0)	6.56(-0)	1.91(-0)	5.23(-1)	1.64(-0)	5.11(-1)	2.22(-1)	6.66(-1)	2.16(-1)
1.08	2.58(0)	6.42(-0)	2.53(-0)	6.83(-1)	1.59(-0)	6.68(-1)	2.89(-1)	6.44(-1)	2.82(-1)
1.16	3.20(0)	6.10(-0)	3.03(-0)	8.37(-1)	1.49(-0)	7.88(-1)	3.51(-1)	6.30(-1)	3.30(-1)
1.32	3.63(0)	5.52(-0)	3.28(-0)	9.25(-1)	1.33(-0)	8.32(-1)	3.84(-1)	5.34(-1)	3.44(-1)
1.64	3.60(0)	4.60(-0)	3.06(-0)	8.90(-1)	1.09(-0)	7.46(-1)	3.65(-1)	4.35(-1)	3.04(-1)
2.28	3.06(0)	3.45(-0)	2.53(-0)	7.30(-1)	7.97(-1)	5.92(-1)	2.96(-1)	3.17(-1)	2.37(-1)
3.56	2.22(0)	2.32(-0)	1.88(-0)	5.13(-1)	5.22(-1)	4.26(-1)	2.05(-1)	2.06(-1)	1.68(-1)
6.12	1.42(0)	1.42(0)	1.26(-0)	3.18(-1)	3.11(-1)	2.75(-1)	1.26(-1)	1.22(-1)	1.08(-1)
11.24	8.39(-1)	8.10(-1)	7.62(-1)	1.82(-1)	1.73(-1)	1.63(-1)	7.10(-2)	6.73(-1)	6.30(-2)
21.48	4.68(-1)	4.45(-1)	4.32(-1)	9.91(-2)	9.30(-2)	9.00(-2)	3.83(-2)	3.58(-2)	3.47(-2)
41.96	2.54(-1)	2.39(-1)	2.36(-1)	5.25(-2)	4.88(-2)	4.81(-2)	2.01(-2)	1.86(-2)	1.84(-2)

SODIUM

3s-7p

3s-4s

3s-5s

EPSIL = 1.76 (-1)

EPSIL = 1.17 (-1)

EPSIL = 1.51 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	8.65(-2)	3.47(-1)	8.38(-2)	1.27(0)	6.92(-1)	1.32(-0)	2.25(-1)	4.60(-1)	2.32(-1)
1.04	1.17(-1)	3.41(-1)	1.14(-1)	1.75(0)	1.70(0)	1.81(-0)	3.08(-1)	5.70(-1)	3.14(-1)
1.08	1.52(-1)	3.30(-1)	1.48(-1)	2.33(0)	2.83(0)	2.39(-0)	4.09(-1)	6.89(-1)	4.12(-1)
1.16	1.84(-1)	3.08(-1)	1.73(-1)	2.96(0)	3.89(0)	2.89(-0)	5.15(-1)	7.89(-1)	4.90(-1)
1.32	2.01(-1)	2.73(-1)	1.78(-1)	3.47(0)	4.57(0)	3.23(-0)	5.96(-1)	8.29(-1)	5.37(-1)
1.64	1.90(-1)	2.21(-1)	1.57(-1)	3.58(0)	4.54(0)	3.19(-0)	6.06(-1)	7.67(-1)	5.24(-1)
2.28	1.53(-1)	1.61(-1)	1.21(-1)	3.15(0)	3.76(0)	2.82(-0)	5.21(-1)	6.10(-1)	4.58(-1)
3.56	1.06(-1)	1.04(-1)	8.54(-2)	2.32(0)	2.63(0)	2.17(-0)	3.76(-1)	4.17(-1)	3.46(-1)
6.12	6.47(-2)	6.13(-2)	5.43(-2)	1.47(0)	1.61(0)	1.44(-0)	2.35(-1)	2.52(-1)	2.27(-1)
11.24	3.65(-2)	3.38(-2)	3.17(-2)	8.43(-1)	9.00(-1)	8.51(-1)	1.33(-1)	1.40(-1)	1.32(-1)
21.48	1.96(-2)	1.79(-2)	1.73(-2)	4.53(-1)	4.78(-1)	4.66(-1)	7.11(-2)	7.40(-2)	7.21(-2)
41.96	1.03(-2)	9.30(-3)	9.16(-3)	2.35(-1)	2.46(-1)	2.44(-1)	3.68(-2)	3.81(-2)	3.77(-2)

SODIUM

3s-6s

3s-7s

3s-3d

EPSIL = 1.66 (-1)

EPSIL = 1.73 (-1)

EPSIL = 1.33 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	8.02(-2)	1.96(-1)	8.40(-2)	3.94(-2)	1.00(-1)	4.07(-2)	1.94(0)	0.0	1.80(-0)
1.04	1.10(-1)	2.30(-1)	1.14(-1)	5.40(-2)	1.16(-1)	5.50(-2)	2.67(0)	0.0	2.46(-0)
1.08	1.46(-1)	2.65(-1)	1.48(-1)	7.16(-2)	1.31(-1)	7.17(-2)	3.60(0)	0.0	3.28(-0)
1.16	1.83(-1)	2.94(-1)	1.76(-1)	8.99(-2)	1.44(-1)	8.46(-2)	4.62(0)	0.0	4.02(-0)
1.32	2.11(-1)	3.01(-1)	1.91(-1)	1.03(-1)	1.46(-1)	9.19(-2)	5.49(0)	0.0	4.60(-0)
1.64	2.14(-1)	2.73(-1)	1.86(-1)	1.04(-1)	1.32(-1)	8.93(-2)	5.76(0)	4.00(-0)	4.70(-0)
2.28	1.83(-1)	2.15(-1)	1.62(-1)	8.87(-2)	1.03(-1)	7.75(-2)	5.13(0)	4.50(-0)	4.25(-0)
3.56	1.31(-1)	1.46(-1)	1.22(-1)	6.34(-2)	6.96(-2)	5.81(-2)	3.82(0)	3.60(-0)	3.31(-0)
6.12	8.17(-2)	8.79(-2)	7.92(-2)	3.94(-2)	4.18(-2)	3.77(-2)	2.44(0)	2.36(-0)	2.22(-0)
11.24	4.61(-2)	4.88(-2)	4.62(-2)	2.22(-2)	2.32(-2)	2.20(-2)	1.40(0)	1.36(-0)	1.31(-0)
21.48	2.46(-2)	2.58(-2)	2.53(-2)	1.18(-2)	1.23(-2)	1.19(-2)	7.56(-1)	7.35(-1)	7.21(-1)
41.96	1.27(-2)	1.33(-2)	1.31(-2)	6.11(-3)	6.30(-3)	6.24(-3)	3.93(-1)	3.82(-1)	3.78(-1)

SODIUM

3s-4d

3s-5d

3s-6d

EPSIL = 1.57 (-1)

EPSIL = 1.69 (-1)

EPSIL 1.75 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	5.45(-1)	0.0	5.11(-1)	2.34(-1)	0.0	2.19(-1)	1.22(-1)	0.0	1.16(-1)
1.04	7.46(-1)	0.0	6.96(-1)	3.19(-1)	0.0	2.98(-1)	1.67(-1)	3.28(-2)	1.57(-1)
1.08	9.92(-1)	0.0	9.16(-1)	4.22(-1)	1.53(-1)	3.92(-1)	2.20(-1)	1.26(-1)	2.06(-1)
1.16	1.25(0)	5.30(-1)	1.11(-0)	5.28(-1)	3.60(-1)	4.69(-1)	2.75(-1)	2.18(-1)	2.46(-1)
1.32	1.44(0)	1.06(-0)	1.23(-0)	6.02(-1)	5.15(-1)	5.14(-1)	3.11(-1)	2.83(-1)	2.67(-1)
1.64	1.46(0)	1.30(-0)	1.20(-0)	6.00(-1)	5.62(-1)	4.94(-1)	3.07(-1)	2.96(-1)	2.54(-1)
2.28	1.25(0)	1.20(-0)	1.04(-0)	5.05(-1)	4.90(-1)	4.89(-1)	2.57(-1)	2.52(-1)	2.14(-1)
3.56	9.01(-1)	8.77(-1)	7.82(-1)	3.59(-1)	3.52(-1)	3.11(-1)	1.81(-1)	1.79(-1)	1.57(-1)
6.12	5.62(-1)	5.51(-1)	5.12(-1)	2.22(-1)	2.18(-1)	2.02(-1)	1.12(-1)	1.10(-1)	1.02(-1)
11.24	3.18(-1)	3.13(-1)	3.00(-1)	1.25(-1)	1.23(-1)	1.18(-1)	6.27(-1)	6.20(-2)	5.93(-2)
21.48	1.70(-1)	1.67(-1)	1.63(-1)	6.65(-2)	6.56(-2)	6.40(-2)	3.33(-2)	3.30(-2)	3.22(-2)
41.96	8.79(-2)	8.65(-2)	8.55(-2)	3.44(-2)	3.39(-2)	3.35(-2)	1.72(-2)	1.71(-2)	1.68(-2)

SODIUM

3s-7d

EPSIL = 1.79 (-1)

N	BORN(1)	BETHE	OCHKUR
1.02	7.31(-2)	0.0	6.89(-2)
1.04	9.97(-2)	3.86(-2)	9.35(-2)
1.08	1.31(-1)	8.92(-2)	1.23(-1)
1.16	1.63(-1)	1.38(-1)	1.46(-1)
1.32	1.84(-1)	1.72(-1)	1.58(-1)
1.64	1.81(-1)	1.75(-1)	1.49(-1)
2.28	1.50(-1)	1.48(-1)	1.25(-1)
3.56	1.06(-1)	1.05(-1)	9.16(-2)
6.12	6.48(-2)	6.42(-2)	5.91(-2)
11.24	3.64(-2)	3.60(-2)	3.44(-2)
21.48	1.94(-2)	1.92(-2)	1.87(-2)
41.96	9.97(-3)	9.88(-3)	9.76(-3)

POTASSIUM

4s-5p

4s-6p

4s-7p

EPSIL = 1.13 (-1)

EPSIL = 1.32 (-1)

EPSIL = 1.42 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	2.24(0)	1.13(+1)	2.19(0)	5.92(-1)	2.72(0)	5.78(-1)	2.51(-1)	1.09(0)	2.44(-1)
1.04	3.06(0)	1.12(+1)	2.98(0)	8.05(-1)	2.67(0)	7.81(-1)	3.40(-1)	1.07(0)	3.30(-1)
1.08	4.03(0)	1.09(+1)	3.90(0)	1.06(0)	2.59(0)	1.01(0)	4.44(-1)	1.04(0)	4.26(-1)
1.16	5.01(0)	1.03(+1)	4.63(0)	1.29(0)	2.42(0)	1.18(0)	5.42(-1)	9.68(-1)	4.92(-1)
1.32	5.69(0)	9.20(0)	5.00(0)	1.44(0)	2.14(0)	1.24(0)	5.99(-1)	8.55(-1)	5.11(-1)
1.64	5.57(0)	7.60(0)	4.74(0)	1.40(0)	1.74(0)	1.14(0)	5.76(-1)	6.92(-1)	4.62(-1)
2.28	4.84(0)	5.63(0)	4.02(0)	1.16(0)	1.27(0)	9.30(-1)	4.70(-1)	5.01(-1)	3.72(-1)
3.56	3.32(0)	3.73(0)	3.02(0)	8.21(-1)	8.24(-1)	6.74(-1)	3.28(-1)	3.24(-1)	2.67(-1)
6.12	2.25(0)	2.25(0)	2.00(0)	5.11(-1)	4.86(-1)	4.33(-1)	2.02(-1)	1.90(-1)	1.70(-1)
11.24	1.32(0)	1.27(0)	1.20(0)	2.92(-1)	2.70(-1)	2.53(-1)	1.14(-1)	5.01(-1)	9.82(-2)
21.48	7.34(-1)	6.90(-1)	6.71(-1)	1.59(-1)	1.43(-1)	1.39(-1)	6.17(-2)	3.24(-1)	5.35(-2)
41.96	3.97(-1)	3.66(-1)	3.62(-1)	8.44(-2)	7.43(-2)	7.34(-2)	3.24(-2)	1.90(-1)	2.81(-2)

POTASSIUM

4s-5s

EPSIL = 9.58 (-2)

4s-6s

EPSIL = 1.25 (-1)

4s-7s

EPSIL = 1.38 (-1)

N	BORN (1)	BETHE	OCHKUR	BORN (1)	BETHE	OCHKUR	BORN (1)	BETHE	OCHKUR
1.02	1.66(0)	0.0	1.91(0)	2.90(-1)	5.38(-1)	3.24(-1)	1.01(-1)	2.58(-1)	1.17(-1)
1.04	2.29(0)	9.14(-1)	2.60(0)	4.00(-1)	7.56(-1)	4.39(-1)	1.39(-1)	3.25(-1)	1.57(-1)
1.08	3.09(0)	3.22(0)	3.45(0)	5.38(-1)	9.95(-1)	5.77(-1)	1.87(-1)	3.96(-1)	2.06(-1)
1.16	3.96(0)	5.48(0)	4.19(0)	6.93(-1)	1.21(0)	6.94(-1)	2.41(-1)	4.57(-1)	2.47(-1)
1.32	4.77(0)	7.08(0)	4.79(0)	8.24(-1)	1.32(0)	7.89(-1)	2.88(-1)	4.82(-1)	2.81(-1)
1.64	5.06(0)	7.38(0)	5.00(0)	8.66(-1)	1.26(0)	8.20(-1)	3.02(-1)	4.48(-1)	2.92(-1)
2.28	4.38(0)	6.28(0)	4.66(0)	7.53(-1)	1.01(0)	7.52(-1)	2.67(-1)	3.57(-1)	2.66(-1)
3.56	3.42(0)	4.46(0)	3.69(0)	5.60(-1)	6.98(-1)	5.82(-1)	1.94(-1)	2.44(-1)	2.04(-1)
6.12	2.19(0)	2.75(0)	2.47(0)	3.53(-1)	4.24(-1)	3.83(-1)	1.22(-1)	1.48(-1)	1.34(-1)
11.24	1.26(0)	1.55(0)	1.47(0)	2.01(-1)	2.36(-1)	2.25(-1)	6.90(-2)	8.21(-2)	7.01(-2)
21.48	6.80(-1)	8.22(0)	8.04(-1)	1.08(-1)	1.25(-1)	1.22(-1)	3.59(-2)	4.34(-2)	4.25(-2)
41.96	3.53(-1)	4.24(-1)	4.22(-1)	5.57(-2)	6.45(-2)	6.40(-2)	1.91(-2)	2.24(-2)	2.22(-2)

POTASSIUM

4s-3d

EPSIL = 9.81 (-2)

4s-4d

EPSIL = 1.25 (-1)

4s-5d

EPSIL = 1.38 (-1)

N	BORN (1)	BETHE	OCHKUR	BORN (1)	BETHE	OCHKUR	BORN (1)	BETHE	OCHKUR
1.02	7.64(0)	1.77(+1)	8.27(0)	1.36(0)	0.0	5.91(-1)	4.27(-1)	0.0	5.25(-2)
1.04	1.04(1)	9.86(+1)	1.14(-1)	1.84(0)	0.0	8.38(-1)	5.75(-1)	0.0	8.48(-2)
1.08	1.38(1)	7.84(-1)	1.53(+1)	2.39(0)	1.99(-1)	1.15(0)	7.39(-1)	0.0	1.40(-1)
1.16	1.74(1)	8.50(0)	1.87(+1)	2.88(0)	5.12(-1)	1.46(0)	8.76(-1)	0.0	2.18(-1)
1.32	1.98(1)	1.59(+1)	2.10(+1)	3.11(0)	7.49(-1)	1.64(0)	9.17(-1)	0.0	3.10(-1)
1.64	1.97(1)	1.91(+1)	1.99(+1)	2.87(0)	8.25(-1)	1.37(0)	8.12(-1)	0.0	3.22(-1)
2.28	1.67(1)	1.73(+1)	1.60(+1)	2.23(0)	7.22(-1)	8.45(-1)	6.07(-1)	1.52(-1)	2.47(-1)
3.56	1.20(1)	1.27(+1)	1.14(+1)	1.49(0)	5.20(-1)	4.65(-1)	3.93(-1)	1.68(-1)	1.70(-1)
6.12	7.46(0)	7.98(0)	7.31(0)	8.86(-1)	3.23(-1)	2.75(-1)	2.30(-1)	1.23(-1)	1.15(-1)
11.24	4.23(0)	4.52(0)	4.29(0)	4.88(-1)	1.82(-1)	1.63(-1)	1.25(-1)	7.47(-2)	7.06(-2)
21.48	2.26(0)	2.42(0)	2.35(0)	2.57(-1)	9.70(-2)	2.08(-2)	6.65(-1)	4.12(-2)	3.98(-2)
41.96	1.17(0)	1.25(0)	1.23(0)	1.32(-1)	5.01(-2)	4.83(-2)	3.35(-2)	2.17(-2)	2.13(-2)

POTASSIUM

4s-6d

EPSIL = 1.44 (-1)

N	BORN (1)	BETHE	OCHKUR
1.02	2.08(-1)	0.0	8.01(-3)
1.04	2.80(-1)	0.0	1.72(-2)
1.08	3.59(-1)	0.0	3.76(-2)
1.16	4.23(-1)	0.0	7.39(-2)
1.32	4.39(-1)	0.0	1.28(-1)
1.64	3.86(-1)	1.18(-2)	1.56(-1)
2.28	2.87(-1)	1.01(-1)	1.40(-1)
3.56	1.86(-1)	1.06(-1)	1.06(-1)
6.12	1.08(-1)	7.65(-2)	7.28(-2)
11.24	5.89(-2)	4.62(-2)	4.45(-2)
21.48	3.08(-2)	2.55(-2)	2.49(-2)
41.96	1.58(-2)	1.34(-2)	1.32(-2)

RUBIDIUM

5s-6p

5s-7p

5s-8p

EPSIL = 1.08 (-1)

EPSIL = 1.27 (-1)

EPSIL = 1.36 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	2.47(0)	1.32(+1)	2.36(0)	6.48(-1)	3.29(0)	6.29(-1)	2.79(-1)	1.35(0)	2.68(-1)
1.04	3.37(0)	1.31(+1)	3.20(0)	8.84(-1)	3.25(0)	8.48(-1)	3.80(-1)	1.33(0)	3.60(-1)
1.08	4.47(0)	1.28(+1)	4.20(0)	1.17(0)	3.15(0)	1.10(0)	5.01(-1)	1.28(0)	4.65(-1)
1.16	5.62(0)	1.21(+1)	5.01(0)	1.46(0)	2.96(0)	1.29(0)	6.23(-1)	1.20(0)	5.42(-1)
1.32	6.47(0)	1.10(+1)	5.51(0)	1.67(0)	2.64(0)	1.39(0)	7.08(-1)	1.07(0)	5.76(-1)
1.64	6.68(0)	9.15(0)	5.43(0)	1.68(0)	2.16(0)	1.33(0)	7.06(-1)	8.70(-1)	5.46(-1)
2.28	5.73(0)	6.86(0)	4.81(0)	1.44(0)	1.59(0)	1.14(0)	6.00(-1)	6.35(-1)	4.61(-1)
3.56	4.26(0)	4.60(0)	3.72(0)	1.05(0)	1.04(0)	8.50(-1)	4.33(-1)	4.13(-1)	3.39(-1)
6.12	2.77(0)	2.81(0)	2.51(0)	6.76(-1)	6.21(-1)	5.55(-1)	2.75(-1)	2.45(-1)	2.19(-1)
11.24	1.65(0)	1.60(0)	1.52(0)	3.98(-1)	3.47(-1)	3.28(-1)	1.50(-1)	1.36(-1)	1.28(-1)
21.48	9.29(-1)	8.83(-1)	8.60(-1)	2.22(-1)	1.87(-1)	1.82(-1)	8.86(-2)	7.25(-2)	7.06(-2)
41.96	5.08(-1)	4.74(-1)	4.69(-1)	1.20(-1)	9.81(-2)	9.70(-2)	4.47(-2)	3.78(-2)	3.74(-2)

RUBIDIUM

5s-6s

5s-7s

5s-8s

EPSIL = 9.17 (-2)

EPSIL = 1.20 (-1)

EPSIL 1.32 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	1.80(-1)	0.0	2.00(0)	2.78(-1)	4.80(-1)	3.35(-1)	1.06(-1)	2.54(-1)	1.20(-1)
1.04	2.51(0)	0.0	2.72(0)	3.85(-1)	1.48(-1)	4.54(-1)	1.47(-1)	3.36(-1)	1.62(-1)
1.08	3.38(0)	2.78(0)	3.62(0)	5.22(-1)	1.04(0)	6.01(-1)	1.99(-1)	4.25(-1)	2.14(-1)
1.16	4.38(0)	5.62(0)	4.43(0)	6.81(-1)	1.31(0)	7.31(-1)	2.58(-1)	5.03(-1)	2.60(-1)
1.32	5.27(0)	7.71(0)	5.15(0)	8.25(-1)	1.47(0)	8.50(-1)	3.12(-1)	5.40(-1)	3.03(-1)
1.64	5.64(0)	8.27(0)	5.52(0)	8.81(-1)	1.42(0)	9.11(-1)	3.31(-1)	5.07(-1)	3.25(-1)
2.28	5.10(0)	7.14(0)	5.27(0)	7.88(-1)	1.15(0)	8.52(-1)	2.92(-1)	4.07(-1)	3.02(-1)
3.56	3.84(0)	5.10(0)	4.22(0)	5.83(-1)	7.99(-1)	6.65(-1)	2.14(-1)	2.79(-1)	2.34(-1)
6.12	2.47(0)	3.16(0)	2.84(0)	3.69(-1)	4.86(-1)	4.40(-1)	1.35(-1)	1.69(-1)	1.54(-1)
11.24	1.42(0)	1.78(0)	1.69(0)	2.10(-1)	2.71(-1)	2.58(-1)	7.67(-2)	9.42(-2)	8.98(-2)
21.48	7.66(-1)	9.47(-1)	9.26(-1)	1.13(-1)	1.44(-1)	1.41(-1)	4.10(-2)	4.99(-2)	4.88(-2)
41.96	3.98(-1)	4.89(-1)	4.86(-1)	5.85(-2)	7.42(-2)	7.36(-2)	2.12(-2)	2.57(-2)	2.55(-2)

RUBIDIUM

5s-4d

5s-5d

5s-6d

EPSIL = 8.82 (-2)

EPSIL = 1.17 (-1)

EPSIL 1.31 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	1.04(+1)	0.0	1.15(+1)	1.24(0)	0.0	8.25(-1)	3.38(-1)	0.0	1.32(-1)
1.04	1.43(+1)	0.0	1.59(+1)	1.67(0)	1.43(-1)	1.16(0)	4.65(-1)	0.0	1.96(-1)
1.08	1.88(+1)	1.61(0)	2.13(+1)	2.15(0)	4.94(-1)	1.58(0)	5.83(-1)	0.0	2.85(-1)
1.16	2.35(+1)	1.35(+1)	2.61(+1)	2.58(0)	8.38(-1)	1.96(0)	6.89(-1)	0.0	3.86(-1)
1.32	2.66(+1)	2.28(+1)	2.92(+1)	2.71(0)	1.08(0)	2.13(0)	7.11(-1)	0.0	4.63(-1)
1.64	2.62(+1))	2.65(+1)	2.74(+1)	2.42(0)	1.13(0)	1.73(0)	6.18(-1)	5.08(-2)	4.08(-1)
2.28	2.18(+1)	2.38(+1)	2.18(+1)	1.81(0)	9.59(-1)	1.05(0)	4.62(-1)	1.84(-1)	2.74(-1)
3.56	1.54(+1)	1.73(+1)	1.54(+1)	1.17(0)	6.80(-1)	5.94(-1)	2.91(-1)	1.84(-1)	1.77(-1)
6.12	9.52(0)	1.08(+1)	9.90(0)	6.84(-1)	4.19(-1)	3.58(-1)	1.79(-1)	1.30(-1)	1.18(-1)
11.24	5.36(0)	6.12(0)	5.80(0)	3.72(-1)	2.36(-1)	2.11(-1)	9.29(-2)	7.82(-2)	7.26(-2)
21.48	2.86(0)	3.27(0)	3.17(0)	1.95(-1)	1.25(-1)	1.18(-1)	4.88(-2)	4.30(-2)	4.11(-2)
41.96	1.48(0)	1.69(0)	1.66(0)	9.98(-2)	6.47(-2)	6.25(-2)	2.50(-2)	2.25(-2)	2.20(-2)

RUBIDIUM

5s-7d

EPSIL = 1.38 (-1)

N	BORN(1)	BETHE	OCHKUR
1.02	1.23(-1)	0.0	3.74(-2)
1.04	1.66(-1)	0.0	5.87(-2)
1.08	2.12(-1)	0.0	9.28(-2)
1.16	2.61(-1)	0.0	1.38(-1)
1.32	2.60(-1)	0.0	1.82(-1)
1.64	2.27(-1)	7.54(-3)	1.77(-1)
2.28	1.38(-1)	9.14(-2)	1.33(-1)
3.56	1.10(-1)	9.68(-2)	9.50(-2)
6.12	6.68(-2)	7.01(-2)	6.51(-2)
11.24	3.66(-2)	4.24(-2)	4.01(-2)
21.48	1.93(-2)	2.34(-2)	2.26(-2)
41.96	9.97(-3)	1.23(-2)	1.21(-2)

CESIUM

6s-7p

EPSIL = 9.96 (-2)

6s-8p

EPSIL = 1.17 (-1)

6s-9p

EPSIL = 1.26 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	2.88(0)	1.69(+1)	2.75(0)	7.64(-1)	4.11(0)	7.23(-1)	3.26(-1)	1.67(0)	3.06(-1)
1.04	3.95(0)	1.68(+1)	3.72(0)	1.04(0)	4.05(0)	9.73(-1)	4.44(-1)	1.64(0)	4.11(-1)
1.08	5.25(0)	1.63(+1)	4.88(0)	1.38(0)	3.92(0)	1.26(0)	5.84(-1)	1.58(0)	5.31(-1)
1.16	6.66(0)	1.54(+1)	5.83(0)	1.74(0)	3.67(0)	1.49(0)	7.25(-1)	1.48(0)	6.21(-1)
1.32	7.78(0)	1.39(+1)	6.50(0)	2.00(0)	3.26(0)	1.62(0)	8.20(-1)	1.31(0)	6.72(-1)
1.64	8.04(0)	1.15(+1)	6.56(0)	2.03(0)	2.66(0)	1.60(0)	8.13(-1)	1.06(0)	6.54(-1)
2.28	7.12(0)	8.52(0)	5.90(0)	1.75(0)	1.94(0)	1.38(0)	6.84(-1)	7.70(-1)	5.60(-1)
3.56	5.36(0)	5.66(0)	4.56(0)	1.28(0)	1.26(0)	1.03(0)	4.88(-1)	4.99(-1)	4.11(-1)
6.12	3.53(0)	3.42(0)	3.05(0)	8.24(-1)	7.47(-1)	6.70(-1)	3.06(-1)	2.94(-1)	2.64(-1)
11.24	2.12(0)	1.94(0)	1.83(0)	4.84(-1)	4.15(-1)	3.92(-1)	1.76(-1)	1.62(-1)	1.53(-1)
21.48	1.21(0)	1.05(0)	1.03(0)	2.70(-1)	2.21(-1)	2.16(-1)	9.65(-2)	8.58(-2)	8.36(-2)
41.96	6.66(-1)	5.60(-1)	5.55(-1)	1.46(-1)	1.15(-1)	1.42(-1)	5.14(-2)	4.45(-2)	4.40(-2)

CESIUM

6s-7s

EPSIL = 8.44 (-2)

6s-8s

EPSIL = 1.11 (-1)

6s-9s

EPSIL = 1.23 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	1.83(0)	0.0	2.17(0)	2.93(-1)	3.19(-1)	3.54(-1)	1.02(-1)	2.36(-1)	1.25(-1)
1.04	2.54(0)	0.0	2.96(0)	4.08(-1)	6.99(-1)	4.81(-1)	1.43(-1)	3.52(-1)	1.70(-1)
1.08	3.46(0)	1.56(0)	3.96(0)	5.60(-1)	1.13(0)	6.44(-1)	1.98(-1)	4.79(-1)	2.28(-1)
1.16	4.54(0)	5.75(0)	4.92(0)	7.43(-1)	1.53(0)	8.04(-1)	2.64(-1)	5.95(-1)	2.86(-1)
1.32	5.57(0)	8.97(0)	5.93(0)	9.21(-1)	1.78(0)	9.81(-1)	3.29(-1)	6.59(-1)	3.51(-1)
1.64	6.09(0)	1.01(+1)	6.67(0)	1.01(0)	1.76(0)	1.10(0)	3.59(-1)	6.32(-1)	3.95(-1)
2.28	5.61(0)	8.97(0)	6.58(0)	9.13(-1)	1.45(0)	1.07(0)	3.24(-1)	5.13(-1)	3.77(-1)
3.56	4.27(0)	6.50(0)	5.36(0)	6.81(-1)	1.02(0)	8.44(-1)	2.40(-1)	3.55(-1)	2.96(-1)
6.12	2.76(0)	4.05(0)	3.65(0)	4.34(-1)	6.20(-1)	5.62(-1)	1.52(-1)	2.16(-1)	1.96(-1)
11.24	1.60(0)	2.29(0)	2.17(0)	2.48(-1)	3.47(-1)	3.31(-1)	8.69(-2)	1.20(-1)	1.15(-1)
21.48	8.62(-1)	1.22(0)	1.20(0)	1.33(-1)	1.84(-1)	1.80(-1)	4.69(-2)	6.37(-2)	6.25(-2)
41.96	4.49(-1)	6.31(-1)	6.28(-1)	6.92(-2)	9.50(-2)	9.44(-2)	2.41(-2)	3.28(-2)	3.26(-2)

CESIUM

6s-5d

EPSIL = 6.63 (-2)

6s-6d

EPSIL = 1.03 (-1)

6s-7d

EPSIL = 1.19 (-1)

N	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR	BORN(1)	BETHE	OCHKUR
1.02	1.62(1)	1.24(+1)	1.52(+1)	3.44(-1)	0.0	1.67(-1)	2.76(-2)	0.0	1.17(-1)
1.04	2.21(1)	1.93(+1)	2.13(+1)	4.78(-1)	0.0	2.80(-1)	4.83(-2)	0.0	1.76(-1)
1.08	2.92(1)	2.71(+1)	2.90(+1)	6.53(-1)	0.0	5.39(-1)	8.98(-2)	0.0	2.88(-1)
1.16	3.64(1)	3.42(+1)	3.66(+1)	8.53(-1)	0.0	1.02(0)	1.64(-1)	0.0	4.67(-1)
1.32	4.09(1)	3.82(+1)	4.23(+1)	1.01(0)	0.0	1.91(0)	2.67(-1)	0.0	7.71(-1)
1.64	3.97(1)	3.68(+1)	3.96(+1)	1.04(0)	0.0	2.88(0)	3.54(-1)	5.95(-1)	1.07(0)
2.28	3.22(1)	3.00(+1)	2.92(+1)	9.12(-1)	2.15(0)	3.29(0)	3.70(-1)	1.10(0)	1.14(0)
3.56	2.22(1)	2.08(+1)	1.85(+1)	6.89(-1)	2.80(0)	2.93(0)	3.08(-1)	1.00(0)	9.62(-1)
6.12	1.35(1)	1.27(+1)	1.13(+1)	4.55(-1)	2.14(0)	2.11(0)	2.11(-1)	6.90(-1)	6.65(-1)
11.24	7.52(0)	7.06(0)	6.54(0)	2.68(-1)	1.32(0)	1.30(0)	1.26(-1)	4.08(-1)	3.99(-1)
21.48	3.98(0)	3.74(0)	3.58(0)	1.47(-1)	7.35(-1)	7.27(-1)	6.93(-2)	2.23(-1)	2.20(-1)
41.96	2.05(0)	1.93(0)	1.88(0)	7.70(-2)	3.88(-1)	3.85(-1)	3.64(-2)	1.17(-1)	1.16(-1)

CESIUM

6s-8d

EPSIL = 1.27 (-1)

N	BORN(1)	BETHE	OCHKUR
1.02	2.18(-2)	0.0	6.56(-2)
1.04	3.38(-2)	0.0	9.61(-2)
1.08	5.46(-2)	0.0	1.52(-1)
1.16	8.74(-2)	0.0	2.37(-1)
1.32	1.28(-1)	0.0	3.74(-1)
1.64	1.58(-1)	4.04(-1)	5.00(-1)
2.28	1.57(-1)	5.39(-1)	5.20(-1)
3.56	1.28(-1)	4.56(-1)	4.29(-1)
6.12	8.69(-2)	3.05(-1)	2.92(-1)
11.24	5.17(-2)	1.78(-1)	1.74(-1)
21.48	2.83(-2)	9.67(-2)	9.54(-2)
41.96	1.48(-2)	5.04(-2)	5.00(-2)

b) Inert Gas Excitation Tables

An Inert-gas study such as the Vainshtein work for the Alkali family has not been done until the present work.

Furthermore with the exception of Helium, the literature does not reveal much data either experimental or theoretical. However, since the usefulness of such a study is clear, a systematic calculation of cross-section data for the inert elements is presented here, and comparison with data from the literature is presented where such data has been found.

INERT ELEMENT C-SECTION TABLES

He: 1s - 2p Born, Ochkur, Bethe, Mod. Bethe

1s - 2s Born, Ochkur

1s - 3s Born, Ochkur

Ne: 2p - 3p Born, Ochkur, Bethe, Mod. Bethe

2p - 3p Born, Ochkur

2p - 4s Born, Ochkur

Ar: 3p - 4s Born, Ochkur, Bethe, Mod. Bethe

3p - 4p Born, Ochkur

3p - 3d Born, Ochkur

Kr: 4p - 5s Born, Ochkur, Bethe, Mod. Bethe

4p - 5p Born, Ochkur

4p - 4d Born, Ochkur

Xe: 5p - 6s Born, Ochkur, Bethe, Mod. Bethe

5p - 6p Born, Ochkur

5p - 4d Born, Ochkur

RN: 6p - 7s Born, Ochkur, Bethe, Mod. Bethe

6p - 7p Born, Ochkur

6p - 6d Born, Ochkur

HELIUM

1s - 2p

EPSIL = 7.74(-1)

1s - 2s

EPSIL = 7.38(-1)

1s - 3s

EPSIL = 8.37(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT(1)	BORN	OCHKUR	LIT(2)	BORN	OCHKUR	LIT
1.05	3.22(-2)	2.98(-2)	0.0	0.0	0.0	2.48(-2)	2.48(-2)	2.60(-2)	4.63(-3)	4.65(-3)	
1.10	4.52(-2)	4.06(-2)	0.0	0.0	0.0	3.24(-2)	3.24(-2)	3.40(-2)	6.03(-3)	6.04(-3)	
1.20	6.26(-2)	5.37(-2)	0.0	0.0	0.0	3.96(-2)	4.04(-2)	3.20(-2)	7.33(-3)	7.49(-3)	
1.80	1.02(-1)	8.63(-2)	4.14(-2)	2.12(-1)	1.05(-1)	4.10(-2)	3.97(-2)	0.0	7.43(-3)	7.16(-3)	
2.50	1.08(-1)	9.60(-2)	8.16(-2)	2.00(-1)	1.33(-1)	3.35(-2)	3.08(-2)	0.0	6.00(-3)	5.48(-3)	
5.00	9.20(-2)	8.78(-2)	8.78(-2)	1.43(-1)	1.28(-1)	1.88(-2)	1.70(-2)	0.0	3.33(-3)	3.00(-3)	
10.00	6.54(-2)	6.41(-2)	6.53(-2)	9.10(-2)	9.70(-2)	9.87(-3)	9.23(-3)	0.0	1.74(-3)	1.62(-3)	
15.00	5.12(-2)	5.06(-2)	5.16(-2)	6.83(-2)	7.70(-2)	6.68(-3)	6.36(-3)	0.0	1.17(-3)	1.12(-3)	
20.00	4.25(-2)	4.22(-2)	4.29(-2)	5.52(-2)	6.43(-2)	5.04(-3)	4.86(-3)	0.0	8.86(-4)	8.53(-4)	
30.00	3.22(-2)	3.20(-2)	3.25(-2)	4.06(-2)	0.0	3.39(-3)	3.30(-3)	0.0	5.95(-4)	5.79(-4)	
50.00	2.22(-2)	2.12(-2)	2.25(-2)	2.72(-2)	0.0	2.04(-3)	2.01(-3)	0.0	3.58(-4)	3.53(-4)	
30.00	1.56(-2)	1.55(-2)	1.57(-2)	1.87(-2)	0.0	1.28(-3)	1.27(-3)	0.0	2.25(-4)	2.22(-4)	

(1) Linear Interpolation From "Ochkur, V.I. and V.F. Bratsev, (1965) Opt. Spectry - USSR 19, 274"; Ochkur Approximation

(2) Linear Interpolation From "Marriot, R. in Atomic Collision Processes, M.R.C. McDowell, Ed., Pub. by North-Holland Publ. Co., Amsterdam"; Close-coupling Calculation

NEON

2p - 3s

EPSIL = 6.12(-1)

2p - 3p

EPSIL = 6.83(-1)

3p - 4s

EPSIL = 7.24(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT	BORN	OCHKUR	LIT	BORN	OCHKUR	LIT
1.05	3.07(-3)	2.60(-3)	0.0	0.0		1.06(-3)	9.60(-4)		4.16(-4)	3.45(-4)	
1.10	4.74(-3)	3.87(-3)	0.0	0.0		1.45(-3)	1.27(-3)		6.61(-4)	5.31(-4)	
1.20	7.46(-3)	5.78(-3)	0.0	0.0		1.91(-3)	1.57(-3)		1.07(-3)	8.31(-4)	
1.80	1.58(-2)	1.39(-2)	2.09(-3)	2.27(-1)		2.54(-3)	2.18(-3)		2.34(-3)	2.10(-3)	
2.50	1.83(-2)	1.70(-2)	1.22(-2)	1.73(-1)		2.33(-3)	2.19(-3)		2.68(-3)	2.52(-3)	
5.00	1.68(-2)	1.63(-2)	1.57(-2)	9.54(-2)		1.48(-3)	1.48(-3)		2.41(-3)	2.34(-3)	
10.00	1.23(-2)	1.21(-2)	1.23(-2)	5.18(-2)		8.14(-4)	8.01(-4)		1.74(-3)	1.71(-3)	
15.00	9.77(-3)	9.67(-3)	9.83(-3)	3.61(-2)		5.59(-4)	5.48(-4)		1.37(-3)	1.36(-3)	
20.00	8.16(-3)	8.10(-3)	8.24(-3)	2.79(-2)		4.25(-4)	4.17(-4)		1.14(-3)	1.13(-3)	
30.00	6.23(-3)	6.20(-3)	6.31(-3)	1.94(-2)		2.87(-4)	2.83(-4)		8.67(-4)	8.63(-4)	
50.00	4.33(-3)	4.32(-3)	4.39(-3)	1.22(-2)		1.74(-4)	1.73(-4)		5.99(-4)	5.98(-4)	
80.00	3.05(-3)	3.05(-3)	3.09(-3)	7.97(-3)		1.10(-4)	1.09(-4)		4.21(-4)	4.21(-4)	

ARGON

3p - 4s

3p - 4p

3p - 3d

EPSIL = 4.26(-1)

EPSIL = 4.82(-1)

EPSIL = 5.16(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT	BORN	OCHKUR	LIT	BORN	OCHKUR	LIT
1.05	6.20(-3)	4.96(-3)	0.0	0.0		1.81(-3)	1.50(-3)		2.66(-3)	2.68(-3)	
1.10	1.07(-2)	8.46(-3)	0.0	0.0		2.79(-3)	2.24(-3)		3.42(-3)	3.47(-3)	
1.20	1.91(-2)	1.49(-2)	0.0	0.0		4.30(-3)	3.41(-3)		4.10(-3)	4.29(-3)	
1.80	4.85(-2)	4.37(-2)	0.0	3.08(-1)		7.60(-3)	7.60(-3)		3.91(-3)	3.96(-3)	
2.50	5.89(-2)	5.49(-2)	3.16(-2)	2.58(-1)		7.43(-3)	7.71(-3)		3.04(-3)	2.89(-3)	
5.00	5.69(-2)	5.50(-2)	5.22(-2)	1.62(-1)		4.90(-3)	4.79(-3)		1.59(-3)	1.42(-3)	
10.00	4.30(-2)	4.24(-2)	4.26(-2)	9.62(-2)		2.73(-3)	2.64(-3)		8.01(-4)	7.34(-4)	
15.00	3.45(-2)	3.42(-2)	3.47(-2)	7.00(-2)		1.89(-3)	1.83(-3)		5.35(-4)	5.01(-4)	
20.00	2.90(-2)	2.88(-2)	2.93(-2)	5.56(-2)		1.44(-3)	1.41(-3)		4.01(-4)	3.81(-4)	
30.00	2.23(-2)	2.22(-2)	2.26(-2)	4.00(-2)		9.75(-4)	9.59(-4)		2.67(-4)	2.58(-4)	
50.00	1.56(-2)	1.55(-2)	1.58(-2)	2.62(-2)		5.93(-4)	5.87(-4)		1.61(-4)	1.58(-4)	
80.00	1.10(-2)	1.10(-2)	1.12(-2)	1.77(-2)		3.74(-4)	3.71(-4)		1.01(-4)	9.99(-5)	

KRYPTON

4p - 5s

4p - 5p

4p - 4d

EPSIL = 3.66(-1)

EPSIL = 4.22(-1)

EPSIL = 4.48(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT	BORN	OCHKUR	LIT	BORN	OCHKUR	LIT
1.05	1.14(-2)	9.19(-3)	0.0	0.0		2.04(-3)	1.64(-3)		6.35(-3)	6.44(-3)	
1.10	1.95(-2)	1.54(-2)	0.0	0.0		3.39(-3)	2.70(-3)		8.19(-3)	8.33(-3)	
1.20	3.43(-2)	2.66(-2)	0.0	0.0		5.65(-3)	4.67(-3)		9.77(-3)	1.03(-2)	
1.80	8.58(-2)	7.63(-2)	0.0	3.49(-1)		1.10(-2)	1.16(-2)		9.21(-3)	9.24(-3)	
2.50	1.04(-1)	9.57(-2)	5.66(-2)	3.15(-1)		1.09(-2)	1.14(-2)		7.10(-3)	6.61(-3)	
5.00	1.00(-1)	9.65(-2)	9.19(-2)	2.15(-1)		7.22(-3)	6.96(-3)		3.69(-3)	3.25(-3)	
10.00	7.55(-2)	7.43(-2)	7.49(-2)	1.34(-1)		4.05(-3)	3.90(-3)		1.86(-3)	1.70(-3)	
15.00	6.05(-2)	5.99(-2)	6.08(-2)	9.98(-2)		2.80(-3)	2.72(-3)		1.25(-3)	1.17(-3)	
20.00	5.08(-2)	5.05(-2)	5.13(-2)	8.02(-2)		2.14(-3)	2.09(-3)		9.48(-4)	9.02(-4)	
30.00	3.90(-2)	3.89(-2)	3.95(-2)	5.86(-2)		1.45(-3)	1.43(-3)		6.72(-4)	6.51(-4)	
50.00	2.73(-2)	2.72(-2)	2.77(-2)	3.90(-2)		8.83(-4)	8.74(-4)		3.77(-4)	3.69(-4)	
80.00	1.93(-2)	1.93(-2)	1.96(-2)	2.66(-2)		5.57(-4)	5.53(-4)		1.47(-3)	1.46(-3)	

XENON

5p - 6s

5p - 6p

5p - 5d

EPSIL = 3.06(-1)

EPSIL = 3.58(-1)

EPSIL = 3.70(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT	BORN	OCHKUR	LIT	BORN	OCHKUR	LIT
1.05	1.26(-2)	9.86(-3)	0.0	0.0		2.30(-3)	1.82(-3)		2.36(-2)	2.42(-2)	
1.10	2.34(-2)	1.84(-2)	0.0	0.0		4.31(-2)	3.52(-3)		3.03(-2)	3.14(-2)	
1.20	4.42(-2)	3.50(-2)	0.0	0.0		7.94(-3)	7.13(-3)		3.61(-2)	3.93(-2)	
1.80	1.21(-1)	1.09(-1)	0.0	3.85(-1)		1.68(-2)	1.85(-2)		3.35(-2)	3.50(-2)	
2.50	1.50(-1)	1.38(-1)	7.19(-2)	3.76(-1)		1.68(-2)	1.74(-2)		2.56(-2)	2.42(-2)	
5.00	1.48(-1)	1.43(-1)	1.34(-1)	2.77(-1)		1.13(-2)	1.07(-2)		1.32(-2)	1.15(-2)	
10.00	1.13(-1)	1.11(-1)	1.12(-1)	1.80(-1)		6.35(-3)	6.11(-3)		6.74(-3)	6.12(-3)	
15.00	9.09(-2)	9.01(-2)	9.13(-2)	1.36(-1)		4.40(-3)	4.27(-3)		4.63(-3)	4.33(-3)	
20.00	7.66(-2)	7.61(-2)	7.73(-2)	1.10(-1)		3.36(-3)	3.29(-3)		3.80(-3)	3.62(-3)	
30.00	5.90(-2)	5.88(-2)	5.98(-2)	8.13(-2)		2.28(-3)	2.25(-3)		3.22(-3)	3.14(-3)	
50.00	4.14(-2)	4.13(-2)	4.20(-2)	5.48(-2)		1.39(-3)	1.38(-3)		1.18(-3)	1.15(-3)	
80.00	2.94(-2)	2.93(-2)	2.98(-2)	3.77(-2)		8.77(-4)	8.72(-4)		3.92(-3)	3.91(-3)	

RADON

6p - 7s

EPSIL = 2.51(-1)

6p - 7p

EPSIL = 3.09(-1)

6p - 6d

EPSIL = 3.19(-1)

N	BORN	OCHKUR	BETHE	MODBETHE	LIT	BORN	OCHKUR	LIT	BORN	OCHKUR	LIT
1.05	2.56(-2)	2.04(-2)	0.0	0.0		3.34(-3)	2.64(-3)		4.07(-2)	4.22(-2)	
1.10	4.42(-2)	3.48(-2)	0.0	0.0		6.12(-3)	5.00(-3)		5.25(-2)	5.49(-2)	
1.20	7.83(-2)	6.11(-2)	0.0	0.0		1.11(-2)	9.96(-3)		6.24(-2)	6.91(-2)	
1.80	1.96(-1)	1.75(-1)	0.0	4.98(-1)		2.30(-2)	2.55(-2)		5.76(-2)	6.13(-2)	
2.50	2.35(-1)	2.17(-1)	1.34(-1)	5.00(-1)		2.27(-2)	2.37(-2)		4.38(-2)	4.16(-2)	
5.00	2.25(-1)	2.17(-1)	2.08(-1)	3.78(-1)		1.51(-2)	1.43(-2)		2.27(-2)	1.97(-2)	
10.00	1.69(-1)	1.67(-1)	1.68(-1)	2.48(-1)		8.46(-3)	8.12(-3)		1.19(-2)	1.08(-2)	
15.00	1.35(-1)	1.34(-1)	1.36(-1)	1.88(-1)		5.85(-3)	5.67(-3)		8.29(-3)	7.75(-3)	
20.00	1.14(-1)	1.13(-1)	1.15(-1)	1.53(-1)		4.47(-3)	4.36(-3)		6.43(-3)	6.11(-3)	
30.00	8.72(-2)	8.69(-2)	8.84(-2)	1.13(-1)		3.03(-3)	2.98(-3)		4.94(-3)	4.79(-3)	
50.00	6.09(-2)	6.08(-2)	6.19(-2)	7.66(-2)		1.84(-3)	1.83(-3)		2.74(-3)	2.68(-3)	
80.00	4.31(-2)	4.31(-2)	4.37(-2)	5.28(-2)		1.16(-3)	1.16(-3)		2.25(-3)	2.23(-3)	

2) Discussion

A comparison of the Born calculations for the Alkalis of Vainshtein with the results of the present work reveals agreement in all cases between the two calculations is within 5%.

As expected the incorporation of the exchange effect (by use of the Ochkur approximation) lowers the value of the cross-section. This is shown for a larger number of cases than previously considered with the Ochkur approximation. Furthermore, as expected, agreement between the Ochkur and Born calculations for large values of incident energy is confirmed.

Likewise, the Modified Bethe calculations decrease the peak value of the cross-section as expected.

Although the agreement between the Born and Bethe calculations in the high energy region is to be expected, since this agreement is forced by use of the Bethe cut-off, the 20% agreement in the upper energy region of the peak value (approximately 4 threshold units) confirms that Bethe approximations can be of significant use when calculations must be "quick". (The Bethe calculation is about 10 times faster than the Born calculation.)

For the Alkali tables two serious disagreements with the Vainshtein data were found. For the Li(2s-3s) case the Vainshtein values (as reprinted in Moiseiwitsch (1968)) for the last three energy values are too large by a factor of 10. This appears to be a typographical error since these values would give a "second" peak to the cross-section at 11 threshold energy units. Furthermore, division by 10 brings the Vainshtein values into agreement

with the present Born calculation.

The second discrepancy is of a more serious nature. For the Potassium (4s-4d), (4s-5d), (4s-6d), the Vainshtein data is in serious disagreement with the present calculation. The difference of a factor of two between the Vainshtein Born calculation and my Ochkur calculation led me to perform a Born calculation for the 4s-4d case. The results of this calculation are:

E	1.02	1.08	1.64	2.28
Born(1)	1.36(0)	2.39(0)	3.11(0)	2.23(0)
Born(2)	5.77(-1)	1.00(0)	1.11(0)	8.31(-1)

E	6.12	11.24	21.48	41.96
Born(1)	8.86(-1)	4.88(-1)	2.57(-1)	1.32(-1)
Born(2)	3.28(-1)	1.83(-1)	9.70(-2)	5.11(-2)

This disagreement is peculiar because agreement between the present calculation and other series of the form $ns-(n-1)d$, $ns-nd$, $ns-(n+1)d$ exists. Since other data for this transition was not found, a definitive resolution of the discrepancy does not seem possible. Further, the wave functions used by Vainshtein are not readily available. They are to be found in Vainshtein (1957) which is a journal reference before the A.P.S. began reprinting Russian articles. However, the Sodium paper Vainshtein L. A. (1965) Opt. Spectry. USSR 18, 538 indicates that the wave functions used were found using the "semi-empirical method taking

account of exchange" as discussed in the 1957 reference. The statement of semi-empirical wave functions suggests that perhaps the data Vainshtein used for the K(4d) (5d) (6d) wave functions was erroneous; hence the present work may be more accurate, since the wave functions used are straight-forward solutions of the HFS-equation.

Returning to the tables, the amount of Inert-gas data available from the literature for comparison with the present work was disappointingly small. The goal was to clearly establish the boundaries of accuracy for the present work by the criteria of comparison with the literature for the two extreme cases of the "inert-core active electron assumption". Although an exhaustive comparison of the Inert-gas study with the literature was not possible, the few cases of comparison with the literature do show reasonable agreement.

Therefore, the credibility of this calculation is firmly established by the detailed comparison with the literature for the Alkali study and the few cases available for the Inert study.

The conclusion is that order of magnitude validity for all cases of electron impact excitation of atoms can be expected from this calculation. The results will tend to be in better agreement with experiment for Alkali-like elements, and for elements of small charge. That is, since our assumptions for the cross-section expressions assume Hydrogen-like behavior for all elements, elements more Hydrogen like will give better results.

VII. SAMPLE RESULTS FOR IONIZATION

In this chapter some results of the ionization calculations will be presented. As indicated in earlier discussion the ionization cross-sections are computed by calculating the first six partial-wave cross-sections and adding them together to obtain the total C-section. The tables, and the normal output of the program IONCST, include the partial C-sections and the total C-section for the given incident energy. The limitations of this calculation will be illustrated by some of the results and this limitation examined in the discussion that follows the tables.

1) Tables

As in earlier tables, the energy range N is given in threshold units; the transition energy E_{psil} is in units of twice the Rydberg; and the cross-sections (partial and total) are measured in units of πa_B^2 .

Ionization Cross-Section Tables

Hydrogen	(1s \rightarrow Continuum)
Helium	(1s \rightarrow Continuum)
Lithium	(2s \rightarrow Continuum)
Sodium	(3s \rightarrow Continuum)
Potassium	(4s \rightarrow Continuum)
Rubidium	(5s \rightarrow Continuum)
Cesium	(6s \rightarrow Continuum)

The literature (Lit) data are referenced as follows:

- Lit⁽¹⁾: Peach, G. (1965) Proc. Phys. Soc. 85, 709
 Lit⁽²⁾: Peach, G. (1966) Proc. Phys. Soc. 87, 375

The data given from these sources is graphically interpolated.

HYDROGEN (1s - ION)

EPSIL = .500

N = 2.00

N = 2.50

N = 2.75

ENERGY

LOG N = .301

LOG N = .398

LOG N = .439

Qe	(This Paper)	Lit.	(This Paper)	Lit.	(This Paper)	Lit.
Qo	.118(0)	.10(0)	.119(0)	.10(0)	.169(0)	.10(0)
Q1	.554(0)	.57(0)	.642(0)	.61(0)	.661(0)	.63(0)
Q2	.154(0)	.12(0)	.191(0)	.19(0)	.202(0)	.19(0)
Q3	.222(-1)	.01(0)	.327(-1)	.02(0)	.368(-1)	.02(0)
Q4	.278(-2)	--	.520(-2)	--	.669(-2)	--
Q5	.341(-3)	--	.838(-3)	--	.126(-2)	--
Qt	.851(0)	.80(0)	.991(0)	.92(0)	.108(1)	.94(0)

HELIUM (1s - 10N)

EPSIL = .860

ENERGY	N = 1.25		N = 1.50		N = 1.75	
	LOG	N = .0969	LOG	N = .176	LOG	N = .243
	(This Paper)	Lit(1)	(This Paper)	Lit(1)	(This Paper)	Lit.
Qe						
Qo	.774(-2)	.1(-2)	.159(-1)	.5(-1)	.220(-1)	.6(-1)
Q1	.391(-1)	.3(-1)	.868(-1)	.9(-1)	.127(0)	.13(0)
Q2	.410(-2)	.1(-1)	.109(-1)	.15(-1)	.178(-1)	.19(-1)
Q3	.215(-3)	.1(-2)	.817(-3)	.1(-2)	.167(-2)	.1(-2)
Q4	.883(-5)	--	.548(-4)	--	.150(-3)	--
Q5	.336(-6)	--	.362(-5)	--	.135(-4)	--
Qt	.512(-1)	.6(-1)	.115(0)	.2(0)	.168(0)	.2(0)
*Q (experiment)		.7(-1)		.17(0)		.27(0)

* McDaniel, E. W., J. W. Hooper, D. W. Martin, and D. S. Harmer (1961), Proc. 5th Int. Cont. on Ionization Phenomena in Gases, Vol (Amersterdam, North-Holland), p. 60

HELIUM (1s - ION)

EPSIL = .860

ENERGY	N = 2.00		N = 2.50		N = 2.75	
	LOG	N = .301	LOG	N = .398	LOG	N = .439
	(This Paper)	Lit(1)	(This Paper)	Lit(1)	(This Paper)	Lit(1)
Qe						
Qo	.262(-1)	.1(-1)	.336(-1)	.2(-1)	.178(0)	.21(-1)
Q1	.157(0)	.25(0)	.194(0)	.34(0)	.205(0)	.35(0)
Q2	.239(-1)	.4(-1)	.327(-1)	.5(-1)	.360(-1)	.53(-1)
Q3	.262(-2)	.1(-2)	.445(-2)	.5(-2)	.526(-2)	.5(-2)
Q4	.286(-3)	--	.625(-3)	--	.816(-3)	--
Q5	.318(-4)	--	.918(-4)	--	.139(-3)	--
Qt	.210(0)	.3(0)	.266(0)	.4(0)	.426(0)	.43(0)
*Q		.28(0)		.32(0)		.36(0)

* Loc. Cit.

LITHIUM

EPSIL =

ENERGY	N = 2.00		N = 2.50		N = 2.75	
	LOG	N = .301	LOG	N = .398	LOG	N = .439
	(This Paper)	Lit(1)	(This Paper)	Lit(1)	(This Paper)	Lit(1)
Qe						
Qo	.250(0)	.1(0)	.447(0)	.15(0)	.160(2)	.16(0)
Q1	.822(0)	.6(0)	.779(0)	.58(0)	.844(0)	.56(0)
Q2	.226(1)	.18(1)	.234(1)	.19(1)	.236(1)	.185(1)
Q3	.913(0)	.7(0)	.105(1)	.9(0)	.107(1)	.9(0)
Q4	.196(0)	.15(0)	.268(0)	.2(0)	.292(0)	.23(0)
Q5	.334(-1)	.5(-1)	.576(-1)	.8(-1)	.688(-1)	.90(-1)
Qt	.447(1)	.34(1)	.494(1)	.38(1)	.206(-2)	.38(1)

SODIUM

EPSIL =

ENERGY	N = 2.00		N = 2.50		N = 2.75	
	LOG N = .301		LOG N = .398		LOG N = .439	
	(This Paper)	Lit(2)	(This Paper)	Lit(2)	(This Paper)	Lit(2)
Qe						
Qo	.415(0)	.5(0)	.543(1)	.5(0)	.319(4)	.5(0)
Q1	.690(0)	.4(0)	.105(1)	.5(0)	.420(2)	.55(0)
Q2	.255(1)	.25(1)	.285(1)	.25(1)	.188(2)	.23(1)
Q3	.117(1)	.11(1)	.146(1)	.12(1)	.788(1)	.12(1)
Q4	.270(0)	.2(0)	.381(0)	.3(0)	.861(0)	.3(0)
Q5	.478(-1)	.3(-1)	.822(-1)	.4(-1)	.132(0)	.4(-1)
Qt	.514(1)	.05(1)	.113(2)	.55(1)	.326(4)	.50(1)

POTASSIUM (4s - ION)

EPSIL = .309

	N = 2.00	N = 2.50	N = 2.75
ENERGY	LOG N = .301	LOG N = .398	LOG N = .439
	(This Paper)	(This Paper)	(This Paper)
Qe			
Qo	.113(1)	.123(1)	.155(1)
Q1	.704(0)	.983(0)	.136(1)
Q2	.322(1)	.312(1)	.317(1)
Q3	.235(1)	.252(1)	.253(1)
Q4	.687(0)	.852(0)	.897(0)
Q5	.140(0)	.214(0)	.243(0)
Qt	.823(1)	.892(1)	.975(1)

RUBIDIUM (5s - ION)

EPSIL = .291

N = 2.00

N = 2.50

ENERGY

LOG N = .301

LOG N = .398

	(This Paper)	(This Paper)
Qe		
Qo	.136(1)	.893(4)
Q1	.100(1)	.466(1)
Q2	.328(1)	.230(2)
Q3	.283(1)	.447(2)
Q4	.902(0)	.156(2)
Q5	.193(0)	.881(1)
Qt	.957(1)	.903(4)

CESIUM (6s - ION)

EPSIL = 2.62

N = 2.00

N = 2.50

ENERGY

LOG N = .301

LOG N = .398

Qe	(This Paper)	(This Paper)
Qo	.127(1)	.907(3)
Q1	.203(1)	.300(1)
Q2	.315(1)	.744(1)
Q3	.380(1)	.833(1)
Q4	.142(1)	.366(1)
Q5	.333(0)	.124(1)
Qt	.120(1)	.931(3)

2) Discussion

From earlier discussion recall the following:

The Born-Coulomb approximation used in this calculation uses the coulomb wave final state wave function.

In this calculation the coulomb wave-function is obtained by use of a series that was limited to 30 terms.

As indicated by the tables, the calculation is valid for a certain range of parameters. Beyond the range of parameters the partial cross-sections, and hence the total cross-sections, are invalid. The reason for the limitation to a range of parameters is the computational difficulty in obtaining coulomb wave functions for a wide range of the variables k_F , l_F , r . A review of these computational difficulties was given by Froberg (1955) in Rev. of Mod. Physics 27, 399. He suggested that numerical tables should be generated for an intermediate range of variables. This suggestion led to the tables of coulomb wave functions published by N.B.S. in Abramowitz (1964). This is mentioned to emphasize the difficulties associated with coulomb wave function calculations over large ranges of the variables.

This computational problem is isolated by the use of the subroutine FLNR and satisfactory values of the wave functions are produced for, small values of the arguments l_F , r , k_F . The validity of the calculation in this "small value" range is established by comparison with the literature. The computational problem of the coulomb wave function can be overcome by use of different series expansions to obtain values in other regions of the function

variables. When the subroutine FLNR is modified in this manner, the program will compute ionization cross-sections in a "general" manner.

Let us examine the nature of the "breakdown" of the calculation. The first "spurious" partial cross-section is for lithium Q_0 (2.75). For this energy (2.75), the higher partial cross-sections appear to be valid.

The next dramatic change is the sodium Q_0 (2.50) partial cross-section. All cross-section beyond this appear in error.

As will be indicated further, this problem should be overcome in future research.

VIII. CONCLUSIONS AND FUTURE RESEARCH

The intent of the present research was to provide inexact but reasonable excitation cross-section values for all elements. This has been achieved. The usefulness of these calculations should be to provide order of magnitude cross-sections for all cases to astrophysicists who, in some cases, have been forced to use πa_B^2 (which can be within four orders of magnitude of the actual cross-sections). By selecting the Alkali (best case) and Inert elements (worst case) as examples of the data available from the calculation, it has been shown that the expected range of validity for other cases using this program is an order of magnitude accuracy.

As mentioned in the introduction precise statements as to the accuracy of the cross-section values are difficult since no "bench mark" seems to exist. However, we would expect that the cross-sections here are quite good (within 10%) in the Born tail (threshold energies greater than 30) and could be used by experimentalists for normalization of their relative data.

For this reason, the possibility of publishing standard high energy cross-section tables for the first several transitions for elements below $Z = 50$ will be pursued.

Furthermore, the use of this technique to compute electron-excitation cross-sections for ions will be investigated. It is clear that since these calculations will involve use of coulomb wave functions for the scattering electron, the problem encountered in the ionization calculation of this research will have to be overcome.

The solution of that problem appears, at this stage, to be the use of an integral expression for the coulomb wave function. This will result in a six-fold integration for the final cross-section and such a numerical calculation would be pursued using Monte-Carlo integration techniques.

The calculation of these cross-sections would be motivated by the active interest of the astrophysicists in investigating the same phenomena (nebulae, aurorae, and solar corona, see Page 1) that motivated the present work. Furthermore, these cross-sections are of interest to people doing stellar modeling. (See Athay (1972.))

Since a set of atomic wave functions for a general calculation is readily available, general calculation of other atomic parameters (e.g. oscillator strengths, transition probabilities) may be attempted, and this may prove useful to the "beam-foil" group at The University of Toledo.

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APPENDIXES

APPENDIX I

Notation

Q = cross-section

\vec{r}_i = position vector of i^{th} electron

A = set of quantum numbers for total atom

a = set of quantum numbers for a particular orbital

$\Phi_A(\vec{r}_1 \dots \vec{r}_2)$ = total wave function (including spin) for atom with electrons in a state A

$\Psi_A(\vec{r}_1 \dots \vec{r}_2)$ = total wave function (neglecting spin) for atom with electrons in a state A

$\phi_a(\vec{r}_i)$ = single orbital wave function (including spin) for atom with i^{th} electron in an orbital state

$\psi_a(\vec{r}_i)$ = single orbital wave function (neglecting spin) for atom with i^{th} electron in an orbital state

\vec{r}_0 = this is reserved for the incident electron position vector in the scattering problem

\vec{r}_e = this is reserved for the emitted electron (secondary electron) position vector in the ionization problem

$\epsilon_{ij \dots k}$ = Levi-Chivita symbol (see Landau (1957))

δ_{ij} = Kroneker -delta (see Landau (1957))

APPENDIX II

Atomic Units

There are two sets of atomic units in common use. They are simply related and are based in the attempt to make parameters of interest dimensionless. Recall the Schrödinger Equation in cgs units,

$$\left[-(\hbar^2/2m) \nabla^2 - e^2/r - E_T \right] \Psi_T = 0 \quad (148)$$

Let $a_0 = \hbar^2 / me^2$ and $R_D = 2R_D = me^4 / \hbar^2$

Multiply equation (148) by \hbar^2 / me^4

$$\left[\left(\frac{\hbar^2}{me^4} \right) \left(\frac{\hbar^2}{2m} \right) \nabla^2 - \left(\frac{\hbar^2 e^2}{me^4} \right) \frac{1}{r} - \left(\frac{\hbar^2}{me^4} \right) E_T \right] \Psi_T = 0$$

Then may be written (149)

$$\left[\frac{1}{2} a_0^2 \nabla^2 - \frac{a_0}{r} - E/R_D \right] \Psi_T = 0 \quad (150)$$

Hence, if we measure length in units a_0 and energy in units R (i.e. twice the Rydberg) the wave equation is

$$\left[\frac{1}{2} \nabla^2 - \frac{1}{r} - E_T \right] \Psi = 0 \quad (151)$$

In these units $e = \hbar = m = 1$ (see Landau pg. 116 (1957)) for reference call these atomic units I (A.U.I.)

Alternatively we might multiply equation (148) by $2/R$ and write the wave equation

$$\left[a_0^2 \nabla^2 - \frac{2a_0}{r} - \frac{E_T}{R_D} \right] \Psi_T = 0 \quad (152)$$

Then measuring energy in Rydbergs and length in Bohr radii, the wave equation is

$$\left[\nabla^2 - \frac{2}{r} - E_T \right] \Psi = 0 \quad (153)$$

these are the atomic units (for reference A.U.II) used by some authors.

Notice in (auI) $k = \sqrt{2E}$ but in (au II) $k = \sqrt{E}$.

For all discussions in this paper atomic units I are used. That is

$$\text{Unit of length} = \hbar^2/me^2 = \text{Bohr Radius} = .529 \text{ \AA}$$

$$\text{Unit of energy} = me^4/\hbar^2 = 2 \text{ Rydberg} = 27.2 \text{ eV}$$

Formulae may be obtained by $e = \hbar = m = 1$.

A convention of referring to units A.U.I as "Hartree Units" and units A.U. II as "Atomic Units" appears to be emerging in recent literature. However, many references to "Hartree Units" as "Atomic Units" already exist.

APPENDIX III

3-j Symbol Identity

A standard text for discussions of angular momentum in quantum mechanics is the work of Edmonds (1960). The necessary relationship required will use results cited without proof from this work.

Consider

$$\sum_{m_f m_i} \int d\Omega Y_{\ell_f m_f}^+(\Omega) Y_{\lambda 0}(\Omega) Y_{\ell_i m_i}(\Omega) \int d\Omega' Y_{\ell_f m_f}(\Omega') Y_{\ell_i m_i}^+(\Omega') Y_{\lambda' 0}(\Omega') \quad (154)$$

$$\equiv \sum_{m_f m_i} \langle \ell_f m_f | \lambda 0 | \ell_i m_i \rangle \langle \ell_i m_i | \lambda' 0 | \ell_f m_f \rangle = I(\ell_i \ell_f \lambda \lambda')$$

Edmonds (pg. 63) gives the following integral in terms of the 3-j symbol

$$\int d\Omega Y_{\ell_1 m_1}(\Omega) Y_{\ell_2 m_2}(\Omega) Y_{\ell_3 m_3} = \left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi} \right]^{1/2} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad (155)$$

But

$$Y_{\ell_i m_i}^+(\Omega) = (-1)^{m_i} Y_{\ell_i, -m_i}(\Omega) \quad \text{so}$$

$$\langle \ell_f m_f | \lambda 0 | \ell_i m_i \rangle = (-1)^{m_f} \left[\frac{(2\ell_f+1)(2\lambda+1)(2\ell_i+1)}{4\pi} \right]^{1/2} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \quad (156)$$

then the sum of interest may be written

$$I(\ell_i \ell_f \lambda \lambda') = \left[\frac{(2\ell_f+1)(2\ell_i+1)}{4\pi} \sqrt{(2\lambda+1)(2\lambda'+1)} \right] \begin{pmatrix} \ell_f & \lambda & \ell_i \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \quad (157)$$

$$\times \sum_{m_f m_i} (-1)^{m_i+m_f} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ -m_i & 0 & m_f \end{pmatrix}$$

The 3-j symbol is zero unless $m_1+m_2+m_3 = 0$. Hence, for the sum

$(-1)^{m_i+m_f} = 1$. Consider

$$J = \sum_{m_f m_i} \begin{pmatrix} \ell_f & \lambda & \ell_i \\ -m_f & 0 & m_i \end{pmatrix} \begin{pmatrix} \ell_i & \lambda' & \ell_f \\ -m_i & 0 & m_f \end{pmatrix} \quad (158)$$

Two symmetry properties of the 3-j symbol from pg. 47 are useful.

Property I: An $\begin{bmatrix} \text{even} \\ \text{odd} \end{bmatrix}$ permutation of the columns is equivalent to multiplication by $\begin{bmatrix} +1 \\ -1 \end{bmatrix} j_1+j_2+j_3$.

Property II:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \quad (159)$$

Using Property I:

$$\begin{aligned} J &= \sum_{m_i, m_f} \begin{pmatrix} l_i & l_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \begin{pmatrix} l_i & \lambda' & l_f \\ -m_i & 0 & m_f \end{pmatrix} \\ &= \sum_{m_i, m_f} (-1)^{l_i + \lambda' + l_f} \begin{pmatrix} l_i & l_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \begin{pmatrix} l_i & l_f & \lambda' \\ -m_i & m_f & 0 \end{pmatrix} \end{aligned} \quad (160)$$

Using Property II:

$$\begin{aligned} J &= \sum_{m_i, m_f} (-1)^{l_i + \lambda' + l_f} \begin{pmatrix} l_i & l_f & \lambda \\ m_i & m_f & 0 \end{pmatrix} \begin{pmatrix} l_i & l_f & \lambda' \\ m_i & -m_f & 0 \end{pmatrix} (-1)^{l_i + l_f + \lambda'} \\ &= \sum_{m_i, m_f} \begin{pmatrix} l_i & l_f & \lambda \\ m_i & -m_f & 0 \end{pmatrix} \begin{pmatrix} l_i & l_f & \lambda' \\ m_i & -m_f & 0 \end{pmatrix} \end{aligned} \quad (161)$$

But pg. 47 of Edmonds gives

$$\sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3 \end{pmatrix} = (2j_3 + 1)^{-1} \int_{j_3 j_3'} \int_{m_3 m_3'} \Delta(j_1 j_2 j_3) \quad (162)$$

where $\Delta(j_1 j_2 j_3)$ indicates the triangle rule must be satisfied.

$$\text{So } J = (2\lambda + 1)^{-1} \int_{\lambda \lambda'} \Delta(l_i l_f \lambda) \quad (163)$$

and

$$I = \frac{(2l_f + 1)}{4\pi} \frac{(2l_i + 1)}{4\pi} \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \int_{\lambda \lambda'} \Delta(l_i l_f \lambda) \quad (164)$$

APPENDIX IV

Equivalent Bethe Approximation

In the Modified Bethe discussion it is asserted that the first non-zero term of the series

$$f(\Omega) = \left(-\frac{2}{k^2}\right) \left\{ \int d\vec{r} \psi_f^\dagger(\vec{r}) \left[\sum_{\ell=0}^{\infty} \frac{(i\vec{k} \cdot \vec{r})^\ell}{\ell!} \right] \psi_i(\vec{r}) \right\} = \left\langle f \left| \sum_{\ell} \frac{(i\vec{k} \cdot \vec{r})^\ell}{\ell!} \right| i \right\rangle \quad (165)$$

is identical to the first non-zero term in the series

$$f'(\Omega) = -\left(\frac{1}{2\pi}\right) \int d\vec{r}' \exp(i\vec{k} \cdot \vec{r}') \left\langle f \left| \sum_{\ell} \frac{(r')^\ell}{(\ell!)} P_{\ell}(\cos[\hat{r} \cdot \hat{r}']) \right| i \right\rangle \quad (166)$$

Let us prove this assertion by reducing Eq. (165) to Eq. (166).

Recall the addition theorem (Jackson (1962) pg. 63),

$$P_{\ell}(\cos[\hat{r} \cdot \hat{r}']) = \left(\frac{4\pi}{2\ell+1}\right) \sum_m Y_{\ell m}(\Omega_r) Y_{\ell m}^\dagger(\Omega_{r'}) \quad (167)$$

Applying this identity to Eq. (166) we may write

$$f'(\Omega) = -\frac{1}{2\pi} \sum_{\ell m} \left(\frac{4\pi}{2\ell+1}\right) \left\langle f \left| \int d\vec{r}' Y_{\ell m}(\Omega_r) Y_{\ell m}^\dagger(\Omega_{r'}) \frac{(r')^\ell}{(\ell!)} \exp(i\vec{k} \cdot \vec{r}') \right| i \right\rangle \quad (168)$$

Choose the integration axis such that \vec{k} is along the z-axis and $\vec{k} \cdot \vec{r}' = Kr' \cos\theta'$ then

$$f'(\Omega) = -\frac{1}{2\pi} \sum_{\ell} \left\langle f \left| \left(\frac{4\pi}{2\ell+1}\right) (r)^\ell \sum_m Y_{\ell m}(\Omega_r) \int_0^\infty \frac{dr' r'^2}{(r')^{\ell+1}} \int_{-1}^{+1} d(\cos\theta') \exp(iKr' \cos\theta') \int_0^{2\pi} d\phi' Y_{\ell m}^\dagger(\theta', \phi') \right| i \right\rangle \quad (169)$$

Rewrite the integral over ϕ in Eq. (169) using (Jackson (1962) pg. 65)

$$Y_{\ell m}(\Omega') = \exp(im\phi') P_{\ell}^m(\cos\theta') \left[\frac{(2\ell+1)}{4\pi} \frac{(\ell-m)!}{(\ell+m)!} \right]^{1/2} \quad (170)$$

$$\int_0^{2\pi} d\phi' Y_{\ell m}^\dagger(\theta', \phi') = \left[\frac{(2\ell+1)}{4\pi} \frac{(\ell-m)!}{(\ell+m)!} \right]^{1/2} P_{\ell}^m(\cos\theta') [2\pi \delta_{m0}]$$

Summing over m , Eq. (169) can then be written,

$$f'(\Omega) = \left(-\frac{1}{2\pi}\right) (2\pi) \sum_{\ell} \langle f | \frac{4\pi}{2\ell+1} (r)^\ell Y_{\ell 0}^+(\Omega) \int_0^\infty \frac{dr'}{(r')^{\ell+2}} \times \int_{-1}^{+1} dx P_\ell(x) \exp(iKr'x) \sqrt{\frac{(2\ell+1)}{4\pi}} |i\rangle \quad (171)$$

The integral over dx may be done by use of the following identity

(Abramowitz (1964) pg. 438)

$$j_\ell(Kr') = \left[(-i)^e/2\right] \int_{-1}^{+1} \exp(iKr'x) P_\ell(x) dx \quad (172)$$

where $j_\ell(r)$ is the spherical Bessel function.

Applying Eq. (172) to Eq. (171) we find

$$f'(\Omega) = \sum_{\ell} \left(\sqrt{\frac{4\pi}{(2\ell+1)}}\right) \langle f | Y_{\ell 0}^+(\Omega) (r)^\ell \int_0^\infty \frac{dr'}{(r')^{\ell+1}} (2)(i)^\ell j_\ell(Kr') |i\rangle \quad (173)$$

Let $y = Kr'$, $dy = Kdr'$ then

$$f'(\Omega) = \left(\frac{2}{K^2}\right) \sum_{\ell} \sqrt{\frac{4\pi}{2\ell+1}} \langle f | Y_{\ell 0}^+(\Omega) (iKr)^\ell \int_0^\infty \frac{dy}{y^{\ell+1}} j_\ell(y) |i\rangle \quad (174)$$

From (Abramowitz (1964) pg. 486 we obtain

$$\int_0^\infty t^\mu J_\nu(t) dt = \left[2^\mu \Gamma\left(\frac{\nu+\mu+1}{2}\right)\right] / \left[\Gamma\left(\frac{\nu-\mu+1}{2}\right)\right] \quad (175)$$

For the case $\mu = -(\ell+1/2)$, $\nu = \ell+1/2$. This is

$$\int_0^\infty t^{-(\ell+1/2)} J_{\ell+1/2}(t) dt = (2)^{-(\ell+1/2)} \frac{\Gamma(1)}{\Gamma(\ell+1/2)} = \sqrt{\frac{2}{\pi}} \frac{1}{(2\ell-1)!!} \quad (176)$$

where (Abramowitz (1964) pg. 256)

$$\Gamma(\ell+1/2) = (2\ell-1)!! \quad ; \quad \Gamma(1/2) = 2^{-1/2} \sqrt{\pi} (2\ell-1)!! \quad (177)$$

Then since $j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x)$, Jackson (1964), Eq. (176) may be used to write,

$$\int_0^\infty \frac{dt}{t^{\ell+1}} j_\ell(t) = \sqrt{\frac{\pi}{2}} \int_0^\infty \frac{dt}{\sqrt{t}} \frac{J_{\ell+1/2}(t)}{t^{\ell+1}} = \frac{1}{(2\ell-1)!!} \quad (178)$$

Applying Eq. (178) to Eq. (174) we write,

$$f'(\Omega) = \left(\frac{2}{K^2}\right) \sum_{\ell} \langle f | \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell 0}^+(\Omega) \frac{(iKr)^\ell}{(2\ell-1)!!} |i\rangle \quad (179)$$

But recall (Jackson (1962) pg. 66)

$$Y_{\ell 0}(\Omega) = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos \theta) \quad (180)$$

then $f'(\Omega)$ is

$$f'(\Omega) = \left(\frac{2}{k^2}\right) \sum_{\ell} \langle f | \frac{(ikr)^{\ell} P_{\ell}(\cos \theta)}{(2\ell-1)!!} | i \rangle \quad (181)$$

By choosing our axis of quantization along \vec{k} so that $\vec{k} \cdot \vec{r} = Kr \cos \theta$ we may write Eq. (165) as,

$$f'(\Omega) = \left(-\frac{2}{k^2}\right) \sum_{\ell} \langle f | (ikr)^{\ell} (\cos \theta)^{\ell} / \ell! | i \rangle \quad (182)$$

To continue, recall (Abramowitz (1964) pg. 798)

$$P_{\ell}(\cos \theta) = \sum_{s=0}^{\ell} a_s (\cos \theta)^s \quad (183)$$

Since we are interested in comparing only the first non-zero term in Eq. (181) and Eq. (182) we need only a_0 in series.

From Magnus and Oberhettig pg. 66 the generalized Legendre Polynomial $P_{\ell}^{\mu}(z)$ has the behavior

$$P_{\ell}^{\mu}(z) = \left[\frac{2^{\ell} \Gamma(\ell + 1/2)}{\Gamma(\ell + 1)} \right] z^{\ell} + O(z^{\ell-1}) \left[1 + O(z^{-1}) \right] \quad (184)$$

therefore, recalling Eq. (183)

$$P_{\ell}(z) \xrightarrow{z \rightarrow \infty} \left[\frac{2^{\ell} \Gamma(\ell + 1/2)}{\Gamma(\ell + 1)} \right] z^{\ell} = \frac{2^{\ell} (2^{-\ell}) \sqrt{\pi} (2\ell-1)!!}{\Gamma(\ell + 1)} z^{\ell} \quad (185)$$

Then since $\Gamma(\ell+1) = \ell!$, Eq. (183) is of the form:

$$P_{\ell}(\cos \theta) = \sum_{s=0}^{\ell-1} a_s (\cos \theta)^s + \frac{(2\ell-1)!! (\cos \theta)^{\ell}}{\ell!} \quad (186)$$

Since the matrix elements of all lower powers of $\cos \theta$ are zero by assumption, Eq. (181) becomes:

$$f'(\Omega) = \frac{2}{k^2} \sum_{\ell} \langle f | (ikr)^{\ell} \left[\frac{(2\ell-1)!!}{(2\ell-1)!!} \right] \frac{(\cos \theta)^{\ell}}{\ell!} | i \rangle \quad (187)$$

which agrees with Eq. (182) to within a factor (-1). Since the object to be measured is $Q = \int d\Omega |f(\Omega)|^2$, the Eqs. (187) and (182) are equivalent for our purpose.

APPENDIX V

Partial Wave Analysis

The decomposition of the Born cross-section Q_{born} in terms of partial wave cross-section Q_{born}^{ℓ} , where ℓ refers to components of the incident wave with angular momentum $\sqrt{\ell(\ell+1)}$ proceeds as follows.

The Born scattering amplitude is

$$f_{\text{Born}}(\Omega) = -\frac{1}{2\pi} \int d\vec{r}_0' \exp[i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}_0'] V_{fi}(\vec{r}_0') \quad (188)$$

where \vec{r}_0' is the position vector of the incident electron, and where

$$V_{fi}(\vec{r}_0') = \int d\vec{r} \psi_f^+(\vec{r}) \frac{1}{|\vec{r} - \vec{r}_0'|} \psi_i(\vec{r}) \quad i \neq f \quad (189)$$

Choosing the coordinate system such that \vec{k}_i is along the z-axis we

write the expansions (Jackson (1962) pg. 567),

$$e^{-i\vec{k}_f \cdot \vec{r}_0'} = (4\pi) \sum_{\ell', m'} (-i)^{\ell'} j_{\ell'}(k_f r_0') Y_{\ell' m'}^+(\Omega_{k_f}) Y_{\ell' m'}(\Omega_{r_0'}) \quad (190)$$

and

$$e^{i\vec{k}_i \cdot \vec{r}_0'} = \sum_{\ell'} (i)^{\ell'} j_{\ell'}(k_i r_0') \sqrt{4\pi(2\ell'+1)} Y_{\ell'}(\Omega_{r_0'}) \quad (191)$$

Applying Eq. (190) and Eq. (191) to Eq. (188) we write

$$f_{\text{Born}}(\Omega) = \left(-\frac{1}{2\pi}\right) \int d\vec{r}_0' V_{fi}(\vec{r}_0') (4\pi) \sum_{\ell' \ell'' m'} (i)^{\ell'} (-i)^{\ell''} \sqrt{4\pi(2\ell'+1)} \\ \times Y_{\ell' m'}^+(\Omega_{k_f}) Y_{\ell''}(\Omega_{r_0'}) Y_{\ell'' m''}(\Omega_{r_0'}) j_{\ell'}(k_i r_0') j_{\ell''}(k_f r_0') \quad (192)$$

The wave functions used in the present calculation can be written:

$$\psi_i(\vec{r}) = R_i(r) Y_{\ell_i m_i}(\Omega_r) \quad ; \quad \psi_f^+(\vec{r}) = R_f^+(r) Y_{\ell_f m_f}^+(\Omega_r) \quad (193)$$

and use can be made of expansion (Jackson (1962) pg. 69),

$$\frac{1}{|\vec{r}_0' - \vec{r}|} = 4\pi \sum_{\ell, m} (2\ell+1)^{-1} \left[\frac{r_<^{\ell}}{r_>^{\ell+1}} \right] Y_{\ell m}^+(\Omega_{r_0'}) Y_{\ell m}(\Omega_r) \quad (194)$$

to rewrite Eq. (189) as

$$V_{fi}(\vec{r}_0') = 4\pi \sum_{\ell m} (2\ell+1)^{-1} Y_{\ell m}^+(\Omega_{\vec{r}_0'}) \int_0^\infty r^2 dr \left[\frac{r^2}{r_0'^2} \right] R_f(r) R_i(r) \quad (195)$$

$$\times \int d\Omega_r Y_{\ell_f m_f}^+(\Omega_r) Y_{\ell m}(\Omega_r) Y_{\ell_i m_i}(\Omega_r)$$

Let us define the two integrals in Eq. (195) as

$$R_\ell^{\text{Born}}(r_0') \equiv \int_0^\infty r^2 dr \left[\frac{r^2}{r_0'^2} \right] R_f(r) R_i(r) \quad (196)$$

and

$$\langle \ell_f m_f | \ell m | \ell_i m_i \rangle = \int d\Omega_r Y_{\ell_f m_f}^+(\Omega_r) Y_{\ell m}(\Omega_r) Y_{\ell_i m_i}(\Omega_r) \quad (197)$$

Then applying Eq. (195) to Eq. (192) we may write

$$f_{\text{Born}}(\Omega) = \left(-\frac{1}{2\pi} \right) \sum_{\ell' \ell'' m'} (4\pi)^2 (i)^{\ell'} (-i)^{\ell''} (2\ell+1)^{-1} \sqrt{4\pi(2\ell'+1)}$$

$$\langle \ell_f m_f | \ell m | \ell_i m_i \rangle Y_{\ell'' m''}^+(\Omega_{\vec{r}_0'}) \int r_0'^2 dr_0' \left[R_\ell^{\text{Born}}(r_0') j_{\ell'}(k_F r_0') \right. \quad (198)$$

$$\left. \times j_{\ell''}(k_F r_0') \right] \langle \ell m | \ell' 0 | \ell'' m'' \rangle$$

where our last term is defined in a manner analogous to Eq. (197).

To simplify the algebra that follows, we define the quantities

$$C(\ell, \ell', \ell'') \equiv (i)^{\ell'} (-i)^{\ell''} (2\ell+1)^{-1} \sqrt{4\pi(2\ell'+1)} \quad (199)$$

$$P(\ell, \ell', \ell'', i, f) \equiv \int_0^\infty r_0'^2 dr_0' R_\ell^{\text{Born}}(r_0') j_{\ell'}(k_F r_0') j_{\ell''}(k_F r_0') \quad (200)$$

and rewrite as,

$$f_{\text{Born}}(\Omega) = -(\partial\pi) \sum_{\ell' \ell'' m'} C(\ell \ell' \ell'') \langle \ell_f m_f | \ell m | \ell_i m_i \rangle \quad (201)$$

$$\times P(\ell, \ell', \ell'', i, f) \langle \ell m | \ell' 0 | \ell'' m'' \rangle Y_{\ell'' m''}^+(\Omega_{\vec{r}_0'}) \quad (202)$$

To obtain the cross-section we require

$$\begin{aligned}
|f_{\text{Born}}(\Omega)|^2 = & \sum_{\substack{\ell' \ell'' m'' \\ \ell m}} \sum_{\substack{L' L'' M'' \\ LM}} C(\ell \ell' \ell'') C^\dagger(L L' L'') \langle \ell_f m_f | \ell m | \ell_i m_i \rangle \langle \ell_i m_i | L M | \ell_f m_f \rangle \\
& \times P(\ell \ell' \ell'' i f) P(L L' L'' i f) [6 + \pi^2] \\
& \times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L'' M'' | L' o | L M \rangle Y_{\ell'' m''}^+(\Omega_{K_F}) Y_{L'' M''}(\Omega_{K_F}) .
\end{aligned} \quad (203)$$

Since we are interested in transitions $Q(n\ell \rightarrow n'\ell')$ we can average the above over m_i and sum over m_f the result of which we indicate by the prime

$$\begin{aligned}
|f'_{\text{Born}}(\Omega)|^2 = & \left(\frac{6 + \pi^2}{2\ell_i + 1} \right) \sum_{\substack{\ell' \ell'' m'' \\ \ell m}} \sum_{\substack{L' L'' M'' \\ LM}} C(\ell \ell' \ell'') C^\dagger(L L' L'') P(\ell \ell' \ell'' i f) P(L L' L'' i f) \\
& \times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L'' M'' | L' o | L M \rangle \\
& \times \sum_{m_i m_f} \langle \ell_f m_f | \ell m | \ell_i m_i \rangle \langle \ell_i m_i | L M | \ell_f m_f \rangle \\
& \times Y_{\ell'' m''}^+(\Omega_{K_F}) Y_{L'' M''}(\Omega_{K_F})
\end{aligned} \quad (204)$$

Using the results of Appendix III to sum over m_i, m_f

$$\begin{aligned}
|f'_{\text{Born}}(\Omega)|^2 = & \left(\frac{6 + \pi^2}{2\ell_i + 1} \right) \sum_{\substack{\ell' \ell'' m'' \\ \ell m}} \sum_{\substack{L' L'' M'' \\ LM}} C(\ell \ell' \ell'') C^\dagger(L L' L'') P(\ell \ell' \ell'' i f) P(L L' L'' i f) \\
& \times \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L'' M'' | L' o | L M \rangle \\
& \times Y_{\ell'' m''}^+(\Omega_{K_F}) Y_{L'' M''}(\Omega_{K_F}) \\
& \times \frac{(2\ell_i + 1)(2\ell_i + 1)}{4\pi} \left(\begin{smallmatrix} \ell_i & \ell_i & \ell \\ o & o & o \end{smallmatrix} \right)^2 \delta_{\ell \ell'} \delta_{m m'}
\end{aligned} \quad (205)$$

Finally after summing over L and M , the above can be written

$$\begin{aligned}
|f'_{\text{Born}}(\Omega)|^2 = & (16\pi)(2\ell_i + 1) \sum_{\substack{\ell' \ell'' m'' \\ \ell m}} \sum_{\substack{L' L'' M'' \\ LM}} C(\ell \ell' \ell'') C^\dagger(L L' L'') P(\ell \ell' \ell'' i f) \\
& \times P(L L' L'' i f) \langle \ell m | \ell' o | \ell'' m'' \rangle \langle L'' M'' | L' o | \ell m \rangle \\
& \times \left(\begin{smallmatrix} \ell_i & \ell_i & \ell \\ o & o & o \end{smallmatrix} \right)^2 Y_{\ell'' m''}^+(\Omega_{K_F}) Y_{L'' M''}(\Omega_{K_F})
\end{aligned} \quad (206)$$

The cross-section is then:

$$\begin{aligned}
Q_{\text{Born}} &= \left[\frac{K_F}{K_I} \right] \int d\Omega_{K_F} |f'_{\text{Born}}(\Omega_{K_F})|^2 = (16\pi)(2l_f+1) \left[\frac{K_F}{K_I} \right] \\
&\times \sum_{l''l'm''} \sum_{l'l'm'} C(l l' l'') C^+(l l' l'') P(l l' l''; i, f) P(l l' l''; i, f) \\
&\times \langle l m | l' 0 | l'' m'' \rangle \langle l'' m'' | l' 0 | l m \rangle \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\times \left[\int d\Omega_{K_F} Y_{l'' m''}^+(\Omega_{K_F}) Y_{l' m'}(\Omega_{K_F}) = \delta_{l'' l'} \delta_{m'' m'} \right]
\end{aligned} \tag{207}$$

The sums over $l''m''$ and l' can be carried out explicitly to give the results

$$\begin{aligned}
Q_{\text{Born}} &= (16\pi)(2l_f+1) \left[\frac{K_F}{K_I} \right] \sum_{l'l''} \sum_{l'} C(l l' l'') C^+(l l' l'') \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&\times P(l l' l''; i, f) P(l l' l''; i, f) \left[\sum_{m m''} \langle l m | l' 0 | l'' m'' \rangle \langle l'' m'' | l' 0 | l m \rangle = \frac{(2l+1)(2l''+1)}{4\pi} \int d\Omega_{l'} \begin{pmatrix} l l' l'' \\ 0 0 0 \end{pmatrix}^2 \right] \\
&= (16\pi)(2l_f+1) \left[\frac{K_F}{K_I} \right] \sum_{l'l''} |C(l l' l'')|^2 |P(l l' l''; i, f)|^2 \\
&\times \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l l' l'' \\ 0 0 0 \end{pmatrix}^2 \frac{(2l+1)(2l''+1)}{4\pi}
\end{aligned} \tag{208}$$

Recalling the definitions of $C(l l' l'')$ and $P(l l' l''; k_i k_f)$, Q_{Born} can be written

$$\begin{aligned}
Q_{\text{Born}} &= (4)(2l_f+1) \left[\frac{K_F}{K_I} \right] \sum_{l'l''} \frac{4\pi(2l'+1)}{(2l+1)^2} (2l+1)(2l''+1) \\
&\times \begin{pmatrix} l_f & l_i & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l l' l'' \\ 0 0 0 \end{pmatrix}^2 \left[\int_0^\infty dr_0 (r_0)^2 \mathcal{R}_l^{\text{Born}}(r_0') j_{l'}(K_I r_0) j_{l''}(K_F r_0) \right]^2
\end{aligned} \tag{209}$$

where, as defined above,

$$\mathcal{R}_l^{\text{Born}}(r_0') \equiv \int_0^\infty r^2 dr \left[\frac{r_c}{r} \right]^{l+1} R_f(r) R_i(r)$$

Since l' is defined in Eq. (191) to refer to the incident electron, the partial cross-section corresponding to incident electrons with angular momentum $\sqrt{l'(l'+1)}$ and scattered electrons with all possible values of angular momentum is,

$$Q_{Born}^{l'} = (16\pi)(2l_f + 1) \left[\frac{K_F}{K_z} \right] \sum_{ll''} \frac{(2l' + 1)(2l'' + 1)}{(2l + 1)} \begin{pmatrix} l_f l_i l' \\ 0 0 0 \end{pmatrix}^2 \quad (210)$$

$$\times \begin{pmatrix} l l' l'' \\ 0 0 0 \end{pmatrix}^2 \int_0^\infty dr'_0 r'^2_0 \mathcal{P}_l^{Born}(r'_0) j_{l'}(K_z r'_0) j_{l''}(K_F r'_0) .$$

NOTE: The presence of a 3j-symbol in an expression such as

$\sum_{l_3=0}^{\infty} \begin{pmatrix} l_1 l_2 l_3 \\ 0 0 0 \end{pmatrix} f(l_1 l_2 l_3)$ implies the triangle condition and reduces the sum range from $l_3 = 0, \infty$ to $l_3 = |l_1 - l_2|, \dots, |l_1 + l_2|$, (Edmonds (1960)

pg. 45).

APPENDIX VI

Ochkur Expression of $f_E(\Omega)$

Recall from our discussion in Chapter III, Section 5, the Born-Oppenheimer approximation to the exchange scattering amplitude for a Helium-like target is written

$$f_E = \left(\frac{1}{2\pi}\right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) e^{-i\vec{K}_F \cdot \vec{r}_1} \left[\frac{1}{|\vec{r}_0 - \vec{r}_1|} - \frac{2}{r_0} + \frac{1}{|\vec{r}_0 - \vec{r}_1|} \right] \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K}_I \cdot \vec{r}_0} \quad (211)$$

Let us break this up into three terms

$$f_1 = \left(\frac{1}{2\pi}\right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) e^{-i\vec{K}_F \cdot \vec{r}_1} \left[\frac{1}{|\vec{r}_0 - \vec{r}_1|} \right] \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K}_I \cdot \vec{r}_0} \quad (212)$$

$$f_2 = \left(\frac{1}{2\pi}\right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) e^{-i\vec{K}_F \cdot \vec{r}_1} \left[\frac{1}{|\vec{r}_0 - \vec{r}_1|} \right] \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K}_I \cdot \vec{r}_0} \quad (213)$$

$$f_3 = \left(\frac{1}{2\pi}\right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) e^{-i\vec{K}_F \cdot \vec{r}_1} \left[-\frac{2}{r_0} \right] \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K}_I \cdot \vec{r}_0} \quad (214)$$

Consider the first term

$$\begin{aligned} f_1 &= \left(\frac{1}{2\pi}\right) \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \Psi_F^\dagger(\vec{r}_2, \vec{r}_0) e^{-i\vec{K}_F \cdot \vec{r}_1} \left[\frac{1}{|\vec{r}_0 - \vec{r}_1|} \right] \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K}_I \cdot \vec{r}_0} \\ &= \left(\frac{1}{2\pi}\right) \int d\vec{r}_1 d\vec{r}_2 \Psi_I(\vec{r}_1, \vec{r}_2) I_F(\vec{r}_1, \vec{r}_2) \exp[i\vec{K} \cdot \vec{r}_2] \end{aligned} \quad (215)$$

where $\vec{K} \equiv \vec{K}_I - \vec{K}_F$ and

$$I_F(\vec{r}_1, \vec{r}_2) = \int d\vec{r}_0 \Psi_F(\vec{r}_2, \vec{r}_0) \frac{\exp[i\vec{K}_I \cdot (\vec{r}_0 - \vec{r}_1)]}{|\vec{r}_0 - \vec{r}_1|} \quad (216)$$

Let us evaluate I_F . Introducing the notation $\vec{r}_{01} = \vec{r}_0 - \vec{r}_1$ let us change variables from \vec{r}_0 to \vec{r}_{01}

$$\begin{aligned}
I_F(\vec{r}_1, \vec{r}_2) &= \int r_0^2 dr_0 d(\cos \theta_0) d\phi_0 \frac{\bar{\Psi}_F^\dagger(\vec{r}_2, \vec{r}_0) e^{i\vec{k}_2 \cdot \vec{r}_0}}{r_{01}} \\
&= \int r_{01} dr_{01} d(\cos \theta_{01}) d\phi_{01} \Psi_F(\vec{r}_2, \vec{r}_1, \vec{r}_{01}) e^{iK_I r_{01} \cos \theta_{01}}
\end{aligned} \quad (217)$$

Defining $X = \cos \theta_{01}$

$$I_F(\vec{r}_1, \vec{r}_2) = \int r_{01} dr_{01} dX \Phi_F(\vec{r}_2, \vec{r}_1, r_{01}, X) e^{iK_I r_{01} X} \quad (218)$$

where

$$\Phi_F(\vec{r}_2, \vec{r}_1, r_{01}, X) = \int d\phi_{01} \Psi_F(\vec{r}_2, \vec{r}_1 + \vec{r}_{01}) \quad (219)$$

(The use of ϕ here does not imply the total wave function including spin.) Let us integrate by parts with respect to X and with respect to r_{01} and neglect each time terms of higher order of smallness.

We obtain

$$I_F(\vec{r}_1, \vec{r}_2) = \frac{1}{iK_F} \int_0^\infty dr_{01} \left[\Phi_F(\vec{r}_2, \vec{r}_1, r_{01}, 1) e^{iK_F r_{01}} - \Phi_F(\vec{r}_2, \vec{r}_1, r_{01}, -1) e^{-iK_F r_{01}} \right] + \dots \quad (220)$$

Noting that

$$\Phi_F(\vec{r}_2, \vec{r}_1, r_{01}, X) \xrightarrow{r_{01} \rightarrow \infty} 0 \quad (221)$$

we write

$$I_F(\vec{r}_1, \vec{r}_2) = -k_I^2 \left[\Phi_F(\vec{r}_2, \vec{r}_1, 0, 1) + \Phi_F(\vec{r}_2, \vec{r}_1, 0, -1) \right] \quad (222)$$

Then since

$$\Phi_F(\vec{r}_2, \vec{r}_1, 0, \pm 1) = 2\pi \bar{\Psi}_F^\dagger(\vec{r}_2, \vec{r}_1) \quad (223)$$

our result is:

$$I_F(\vec{r}_1, \vec{r}_2) = \left[\frac{4\pi}{K_I^2} \right] \bar{\Psi}_F(\vec{r}_2, \vec{r}_1) \quad (224)$$

Ochkur (1964) argues that by a similar calculation it may be shown that

$$f_2 = O(K_I^{-6})$$

$$f_3 = O(K_I^{-6})$$

Therefore, he claims the exchange amplitude f_E , may be approximated

$$\begin{aligned}
 f_E &\approx \frac{4\pi}{K_1^2} \frac{1}{2\pi} \int d\vec{r}_1 d\vec{r}_2 \Psi_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K} \cdot \vec{r}_1} \Psi_F^\dagger(\vec{r}_1, \vec{r}_2) \\
 &= \frac{2}{K_1^2} \int d\vec{r}_1 d\vec{r}_2 \bar{\Psi}_I(\vec{r}_1, \vec{r}_2) e^{i\vec{K} \cdot \vec{r}_1} \bar{\Psi}_F^\dagger(\vec{r}_1, \vec{r}_2) .
 \end{aligned}
 \tag{225}$$

APPENDIX VII

User Manual

This section describes the details of the administration of the computer programs. The three programs used in this work are:

HFSWF; the Herman-Skillman Hartree-Fock-Slater Wave Function program with the modification discussed earlier.

EXCST; the excitation cross-section program with four options (Born, Bethe, Ochkur, Mod. Bethe) for the approximation to the cross-section.

IONCST; the ionization cross-section program that uses the Born-Coulomb approximation.

For each of these programs a sample of the input data in the form to be entered into the computer is given. Note in the examples, following standard Fortran IV usage, a "blank" data value results in the assigning of the value zero to the variable being read (e.g. Read (IR, 10) X, Y, Z with data 10, , 15 assigns the values $x = 10$, $Y = 0$, $Z = 15$).

The input data are discussed in the sequence in which they appear on the data cards of the program. For each data card the format statement number as it appears in the program listing is given as follows:

Data Card #N (Format M).

Finally a sample output is given and briefly discussed

1) HFSWF: Hartree-Fock-Slater Wave Function

A) Sample Input

UNB *
 C FORTACLG,PARM=NOMAP
 *SYSIN DD *
 PROGRAM HFSWF(INPUT)

%MSGLEVEL=(0,0)

A 010
 A 020
 A 030
 A 040
 A 050
 A 060
 A 070
 A 080

=====

*
 * * * HFSWF * * *
 *
 * A FORTRAN PROGRAM TO CALCULATE HARTREE-FOCK-SLATER
 * NUMERICAL WAVE FUNCTIONS AS PUNCHED CARD OUTPUT. *

END
 SUBROUTINE SCHEQ (ZZ,EN,AMBA,NOFI,KKK,MESS,SCF,THRESH)

A 531-
 B 1

END

B 430-

YSIN DD *

TON- 4 CASES

	001	0.00001	521	1	20	1	0	6	6	5	7	1	1
00	.98958	.97892	.96819	.95748	.94688	.93642	.92614	.91604	.90613				
42	.87756	.85941	.84195	.82516	.80902	.79352	.77862	.76430	.75051				
19	.71184	.68796	.66536	.64393	.62355	.60415	.58564	.56796	.55105				
86	.50445	.47648	.45078	.42717	.40540	.38525	.36651	.34902	.33266				
36	.28967	.26547	.24431	.22577	.20943	.19492	.18195	.17029	.15976				
22	.13376	.12024	.10906	.09965	.09154	.08441	.07807	.07238	.06725				
53	.05466	.04811	.04268	.03811	.03424	.03092	.02805	.02778	.02778				
78	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778				
78	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778				
78	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778				
78	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778	.02778				

8 0

2-1030.6

2-135.53

6-123.25

2-19.728

6-15.249

10-7.0975

2-1.9456

6-0.9519

1-.2199

1-.1089

1-.0561

EXHIBIT 1

HFSWF SAMPLE INPUT

B) Input Data Values

Data Card #1 (Format 138)

This card contains heading information. Any 72 characters of information may be put in by the user for a title for his output. In the sample input the title chosen was "Krypton - 4 cases".

Data Card #2 (Format 131)

This card contains the program control information. The parameters are: KEY, TOL, THRESH, IPRATT, MAXIT, NOCOPY, KUT, IP, IM, IR, ID, DEFOLT, JE. The usual values of these parameters for the cross-section calculation are denoted by * *.

KEY: This determines the nature of the starting potential. The allowed values are:

- ** 0; The normalized (1) potential on a 110-point mesh is read in and used to construct the 441-point starting potential. (Suggested normalized potentials are found in Table A at the end of this Manual).
- 1; The starting potential is given in the same format as the unabridged self-consistent potential that is output from the calculation. (i.e. 441 points)
- 2; The starting potential for Z is obtained by a linear extrapolation of the two unabridged potentials for atoms ZE2 and ZE3 where $Z - ZE3 = ZE3 - ZE2$. Both unabridged potentials must be read into the program.

(Note: The options 1 and 2 for the parameter KEY are included because they might be used if a series of elements were to be calculated. In that case the series would be started for the first element with the option KEY = 0, but the self-consistent potential, all 441 points, might be saved and used as the starting potential for the next element in the series. If this were done the option KEY = 1 would be used for the start of the second element).

TOL: This is the tolerance for self-consistency defined as $TOL = \max |rV_o^f(r) - rV_o^f(r)|$. Herman and Skillman (1963) (H.A.S.) note that since tests of TOL = .001, .0001, .00001 yield potentials mutually consistent the first value is suggested.

(1) The normalized potential $U(r)$ is defined. $U(r) = -rV(r)/2Z$

- ** .001; the value found by trial and error to be preferred by H.A.S.
- THRESH: The eigenvalue accuracy criterion defined by
- ** .00001; the value found by H.A.S. to be consistent with TOL = 001
- MESH: The number of points used in the integration mesh for the Schrödinger equation subroutine. (SCHEQ).
- ** 441: The usual value for the integration mesh.
- 481: } These values are used for the highly excited configuration
521: } where orbitals extend out to very large (radial)
 } distances.
- IPRATT: The number of times an improvement scheme due to Pratt (1952) should be used.
- ** 1; Normal value found by trial and error by H.A.S.
- MAXIT: The maximum number of iterations permitted.
- ** 20: Recommended value.
- 30: If for some reason (such as a poor choice of starting potential) a large number of interactions is expected to reach self-consistency, assign this value.
- NOCOPY: This controls the nature of the output
- ** 0: The active electron wave functions are the output.
- 1: The output is the self-consistent potential (441-points) and all radial wave functions.
- KUT: The analytic form of the potential is selected as either a potential computed from the wave functions for the entire range of r , or
- $$V(r) \approx \begin{cases} V_0(r) & r < r_0 \\ -2(Z-N+1)/r & r \gg r_0 \end{cases}$$
- where r_0 is the value of r for which $V_0(r) = -2(Z-N+1)/r$.
- ** 0: The potential is $V(r)$. (This is a restriction of the Slater assumption to the interior region).
- 1: The potential is $V_0(r)$ for all r .

IP,IM,IR,ID: These parameters control the type of device used for input (IR) and output (IP,IM,ID). The allowed devices are:

5 = card reader
 6 = printer
 7 = card punch
 no = some storage device (unit tape or disk).

IR is the input control

IP is the online output information

IM is the total wave functions and the potential control (see NOCOPY)

ID is the active electron wave function control.

** 6,6,5,7; These are the normal input output devices. That is input is punched cards. Output is printer and punched cards.

DEFOLT: This parameter controls whether or not the normal values (denoted above by **) are to be used.

0: Set parameters equal to normal values

1: All parameters are read as input.

JE: The number of excited states to be calculated using the self-consistent potential.

** 1: Normal value

N: Used to produce a set of N excited state wave functions.

Data Card #3 (Format 124)

This card contains the atomic potential. Eleven of these cards are used to read in the starting atomic potential RU2(m) in the normal form of a 110-point mesh.

(See "KEY" discussion above.)

RU2(m): m values from 1 to 441 by 4's. The suggested values for RU2 for all atoms are found in Table A.

Data Card #4 (Format 125)

This card contains information about the configuration of the atom.

Z: The atomic number

NCORES: The number of core (i.e. filled) orbitals.

NVALENCE: The number of valence (i.e. unfilled) orbitals.

ION: The Ionicity (i.e. the net charge) on the atom.

(Note: Although the option of calculating wave functions for ions was not used in the present work the HFSWF program will compute such wave functions.)

Data Card #5 (Format 127)

This card contains orbital information. A set of (NCORES + NVALENCE) of these cards are read (see the sample input). The parameters are:>NNLZ, WWNL, EE.

NNLZ: The principal and orbital quantum numbers.

(Note: $NNLZ = 100n + 10\lambda + c$, where n is the principal quantum number, λ is the angular quantum number and c an integer (0,1,...9) which can be used to distinguish different configurations from one another at the discretion of the user.)

WWNL: The occupation number (i.e. the number of electrons in the orbital).

EE: The starting eigenvalue for the orbital.

Suggested values for>NNLZ, WWNL, and EE are given for ground state configuration in Table A.

Data Card #6 (Format 127)

This card is a special use of the data card #4. The value -1 is assigned to the atomic charge parameter Z . The program interprets $Z = -1$ as signifying the end of the ground state configuration. Control is transferred to the excited state calculation section of the program.

Data Card #7 (Format 127)

This card contains excited state orbital information. This is a series of JE cards (see Data Card 1) containing>NNLZ, WWNL, EE for the excited states. The value of E (in Rydbergs) should be obtained from the C. Moore (1950) table or other reference tables.

The positions of the data for these cards may be seen

from the sample input or read from the appropriate format statements in program listing given in Chapter V, Section 1.

C) Sample Output

For the "normal" values of the parameters discussed above, the output from program HFSWF is of two types:

- 1) The printed output, which gives information about each iteration (see Exhibit 2). The first item is the "title" as discussed above (Data Card #1). The second item is the value of the parameter KEY which indicates the type of starting potential used (as discussed above in Data Card #2).

Next for each iteration the following is printed

ITER = "iteration" number

Z = atomic number

DELTA = measure of self-consistency (when DELTA < .001 calculation stops)

I(DEL) = serial number of mesh point at which self-consistency is poorest

X(DEL) = corresponding value of X

I(CUT) = serial number of mesh point closest to r_0 ,
where $r_0 V_0(r_0) = -2(I_{0N}+1)$

X(CUT) = corresponding value of X

N cards and M cards denote the number of cards that would be produced by a punching of All wave functions in the configuration.

- 2) The punched output which is decks of about 90 cards for each wave function.

For each wave function the first card contains NLZ, XL, EE, WWNL, KKK, according to (Format 142).

NLZ = $100n + 10\lambda + c$; (identical to>NNLZ in Data Card #5 above)

XL = numerical value of λ in floating point form

EE = energy eigenvalue

WWNL = occupation number

KKK = last mesh point for tabular representation of $P(n, \lambda; r)$

Z = atomic charge.

The KKK values of $P_{n\lambda}(r)$ appear in the next $(KKK-1)/5+1$ cards. There are 5 entries per card on the first $(KKK-1)/5$ cards of the set, and a single entry (the KKKth) on the final line in this set. This cycle is then repeated for each of the remaining orbitals.

The serial numbers 1 to KKK have the following values of the true radial distance r associated with them.

Recall $x = r/\mu$

where $\mu = \frac{1}{2} \left(\frac{3\pi}{4} \right)^{2/3} Z^{-1/3}$

The serial numbers refer to the integration mesh (x-mesh) used in the radial wave function integration. It is composed of 11 blocks of 41 points each. Each block has 40 equally spaced intervals.

<u>BLOCK NUMBER</u>	<u>INITIAL X</u>	<u>INTERVAL ΔX</u>	<u>FINAL X</u>	<u>LAST POINT</u>
1	0.0	.0025	.1	41
2	0.1	.005	.3	81
3	.3	.01	.7	121
.
.
11	102.3	2.56	204.7	441

(Note: Any wave functions may be used with programs EXCST and IONCST provided they are scaled into this mesh and arranged into the format of the wave functions output from HFSWF. This was done with the analytic wave functions of hydrogen to test the cross-section programs.)

KRYPTON 4 CASES

KEY = 0

ITER	Z	DELTA	I(DEL)	X(DEL)	I(CUT)	X(CUT)
1	36.	2.0038214E 00	405	112.540	441	204.700
2	36.	1.0018797E 00	402	104.860	270	10.940
3	36.	2.7208328E-03	279	12.380	270	10.940
4	36.	1.3160706E-03	279	12.380	270	10.940
5	36.	4.0054321E-04	270	10.940	270	10.940

NCARDS= 578 MCARDS=14

NCARDS= 578 MCARDS=14

EXHIBIT 2

HFSWF SAMPLE OUTPUT (PRINTED OUTPUT)

410	1.0000000E	00-9.5209509E-01	6.0000000E	00 401 36.		Z 36	1
0.0		7.0760769E-05	2.7964660E-04	6.2165153E-04	1.0918884E-03	Z 36	2
1.6855842E-03		2.3980788E-03	3.2248199E-03	4.1613765E-03	5.2034073E-03	Z 36	3
.							
.							
5.6951222E-10		4.1242476E-10	2.9837133E-10	2.1548405E-10	1.5512808E-10	Z 36	81
1.1100898E-10						Z 36	82
500 0.0		-2.1989995E-01	1.0000000E	00 441 36.		Z 36	1
0.0		2.5549415E-03	4.9868859E-03	7.2991028E-03	9.4948038E-03	Z 36	2
.							
.							
7.8121731E-10						Z 36	90
510 1.0000000E		00-1.0889995E-01	1.0000000E	00 441 36.		Z 36	1
.							
.							
-1.4592098E-07						Z 36	90
420 2.0000000E		00-5.6100000E-02	1.0000000E	00 441 36.		Z 36	1
.							
.							
-2.9764298E-05	-2.4344161E-05	-1.9828294E-05	-1.6053091E-05	-1.2880814E-05		Z 36	89
-1.0194870E-05						Z 36	90

EXHIBIT 3
HFSWF SAMPLE OUTPUT (PUNCHED OUTPUT)

2) EXCST: Excitation Cross-Sections

a) Sample Input

B) Input Data Values

Data Card #1 (Format 46)

This card contains the program control information. The parameters are: N, NTC, NC, NOTP, AQ.

N: This determines the number of energy values to be read into the program.

-1; If this value is used a standard set of energy values is assumed. (See Data Card #2)

NTC: The type of case is indicated by this parameter.

1; A single case (i.e. A cross-section for a single transition in a single approximation is given say Na (3s-3p) in the Bethe approximation.)

2; A multiple approximation for a fixed transition (i.e. For a specific transition Na(3s-3p) the cross-section is calculated in more than one approximation, say the Born and the Bethe approximations.)

3; A multiple excited state function case. (i.e. For a series of excited states, the cross-section is calculated for a specified approximation for each transition say Na(3s-3p), Born; Na(3s-4p), Bethe.)

NC: The number of cases. This should be in agreement with the value of NTC. (i.e. NTC = 1 NC = 1; if NTC = 2 NC = number of approximations used; if NTC = 3 NC = number of excited state wave functions.

NOTP: The type of output format (See sample outputs at end of this section.)

1; Punched Cards

2; Single List

3; Multiple List

AQ: The atomic element name as it will appear in the output. This is limited to an 8 character length (e.g. potassium = potassium).

Data Card #2 (Format 47)

This is the set of incident energy values. These energies are in threshold units of energy. As indicated above

a value of $N = -1$ on Data Card #1 assumes a set of 20 energy values. They are (1.2, 1.35, 1.50, 1.75, 2.00, 2.33, 2.67, 3.0, 3.5, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 12.0, 15.0, 18.0, 21.0, 24.0).

If the $N = -1$ is chosen, no Data Cards #2 are included in the deck.

If $N \neq -1$, the number of values on this card must equal N .

Data Card #3 (Format 48)

This is the first atomic wave function Data Card. It contains information about the ground state wave function the parameters are NLZI, XLI, EEI, WWNLI, KKKI, Z.

NLZI: This is the principal and orbital angular momentum quantum number. (e.g. 3s→30)

XLI: This is the orbital angular momentum quantum number.

EEI: This is the eigenenergy of the orbital.

WWNLI: This is the occupation number (i.e. number of electrons) for the orbital.

KKKI: This is the number of points in the Herman-Skillman mesh used to give the wave function.

Z: This is the atomic number.

Data Card #4 (Format 49)

This card contains 5 of the values of the initial radial wave function. There are $(KKKI-1)/5+1$ of these cards for the initial state wave function. Notice that since the radial wave function is the function $P(nl;r)$ and the boundary condition requires $P = 0$ at $r = 0$, then the first wave function value is always 0.0.

PIN(N): The values of the initial state radial wave function.

Data Card #5 (Format 48)

This is the first final state wave function Data Card. The parameters are NLZ2, XL2, EE2, WWNL2, KKK2, Z. This card is of the same form as Data Card #3 and the parameters are described above.

Data Card #6 (Format 49)

This card contains 5 values of the final state radial wave function. These are $(KKK2-1)/5+1$ of these cards for the final state wave function.

PF(N): The values of the final state radial wave function.

N.B. Cards 5 and 6 are repeated for each of the final states for which cross-sections are to be calculated.

Data Card #7 (Format 51)

This is the approximation specification card. The parameters are: IPROX, BQ.

IPROX: The numeric value of the approximation

- 1; Born Approximation
- 2; Ochkur Approximation
- 3; Bethe Approximation
- 4; Modified Bethe Approximation

BQ: The 8 character abbreviation of the approximation as it will be printed in the output.

C) Sample Output

There are three possible forms for the output. The form used is selected by a choice of the parameter NOTP as discussed above in Section B. Examples for each form follow.

1.200	0.405E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
1.350	0.677E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
1.500	0.825E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
1.750	0.945E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
2.000	0.990E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
2.230	0.100E	03BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
2.670	0.982E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
3.000	0.955E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
3.500	0.907E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
4.000	0.859E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
5.000	0.772E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
6.000	0.699E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
7.000	0.639E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
8.000	0.589E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
10.000	0.511E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
12.000	0.452E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
15.000	0.388E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
18.000	0.341E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
21.000	0.304E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)
24.000	0.276E	02BETHE	(11.)	SODIUM	(30-31)(EPSIL= 0.753E-01)

EXHIBIT 5

EXCST SAMPLE OUTPUT (NOTP = 1)

SODIUM - BE THE

CROSS-SECTIONS ARE IN UNITS OF πa_0^2 (BOHR RADIUS**2).
 INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
 EPSIL IS IN UNITS OF TWICE THE RYDBERG.

(AT. NO. = 11.)

(EPSIL = 7.531E-02)

(NL=N'L':30-31)

*****		*****		*****		*****	
N	SIG(N)	N	SIG(N)	N	SIG(N)	N	SIG(N)

1.200	4.048E 01	1.350	6.766E 01	1.500	8.245E 01		

1.750	9.451E 01	2.000	9.905E 01	2.330	9.997E 01		

2.670	9.824E 01	3.000	9.550E 01	3.500	9.070E 01		

4.000	8.588E 01	5.000	7.716E 01	6.000	6.991E 01		

7.000	6.392E 01	8.000	5.892E 01	10.000	5.109E 01		

12.000	4.524E 01	15.000	3.877E 01	18.000	3.405E 01		

21.000	3.045E 01	24.000	2.759E 01	0.000	1.484E-78		

EXHIBIT 6

EXCST OUTPUT (NOTP = 2)

F 0

(AT.NO.=11.)

CROSS-SECTIONS ARE IN UNITS OF $\pi \times (\text{BOHR RADIUS})^2$.
 INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
 EPSIL IS IN UNITS OF TWICE THE RYDBERG.

N	SIG(N)	SIG(N)	SIG(N)	SIG(N)
1.200	8.584E 01	8.027E 01	4.048E 01	0.0
1.350	9.984E 01	9.062E 01	6.766E 01	0.0
1.500	1.064E 02	9.468E 01	8.245E 01	1.326E 01
1.750	1.101E 02	9.631E 01	9.451E 01	2.607E 01
2.000	1.098E 02	9.598E 01	9.905E 01	3.448E 01
2.330	1.069E 02	9.408E 01	9.997E 01	4.110E 01
2.670	1.029E 02	9.133E 01	9.824E 01	4.397E 01
3.000	9.871E 01	8.860E 01	9.550E 01	4.557E 01
3.500	9.261E 01	8.427E 01	9.070E 01	4.661E 01
4.000	8.701E 01	8.013E 01	8.588E 01	4.664E 01
5.000	7.750E 01	7.262E 01	7.716E 01	4.526E 01
6.000	6.989E 01	6.631E 01	6.991E 01	4.317E 01
9.000	5.437E 01	5.263E 01	5.470E 01	3.681E 01
10.000	5.074E 01	4.930E 01	5.109E 01	3.490E 01
12.000	4.487E 01	4.385E 01	4.524E 01	3.182E 01
15.000	3.842E 01	3.775E 01	3.877E 01	2.804E 01
18.000	3.374E 01	3.326E 01	3.405E 01	2.511E 01
21.000	3.016E 01	2.980E 01	3.045E 01	2.278E 01
24.000	2.732E 01	2.705E 01	2.759E 01	2.088E 01
APPROX. (NL-N'L')	BORN (30-31)	OCHKUR (30-31)	RETHE (30-31)	MODRETHE (30-31)
EPSIL	7.531E-02	7.531E-02	7.531E-02	7.531E-02

EXHIBIT 7
 EXCST SAMPLE OUTPUT (NOTP = 3)

3) IONCST: Ionization Cross-Sections

a) Sample Input

// JOB ' ' , , ' , MSGLEVEL=(0,0)

// EXEC FORTGCLG.PARM='BCD,NOSOURCE'

//FORT.SYSIN DD *

C PROGRAM IONCST(INPUT)

A 1
A 2
A 3
A 4
A 5
A 6
A 7
A 8

C =====
C * * * * IONCST * * * *
C *
C * A FORTRAN PROGRAM TO CALCULATE PARTIAL CROSS-SECTIONS
C * FOR NEUTRAL ATOMS IONIZED BY INCIDENT ELECTRONS *
C *

END
FUNCTION FINR (L,RHO,ETA)

A 204-
B 1

END

G 11-

/*

//GO.SYSIN DD *

HELIUM

100 0.0 -1.7212696E 00 2.0000000E 00 321 2. Z 2 1
0.0 8.4950104E-03 1.6930431E-02 2.5306545E-02 3.3623707E-02 Z 2 2
4.1882206E-02 5.0082348E-02 5.8224466E-02 6.6308796E-02 7.4335754E-02 Z 2 3

6.2946981E-09 4.7294328E-09 3.5502439E-09 2.6611420E-09 1.9896926E-09 Z 2 65
1.4811201E-09 Z 2 66
2.75 BORN

/*

EXHIBIT 8

SAMPLE INPUT IONCST

b) Input Data Values

Data Card #1 (Format 17)

This is a heading card. The 8 character abbreviation for the element as it will appear in the output.

Data Card #2 (Format 18)

This is the initial (bound) state atomic data card. The parameters are: NLZI, XLI, EEI, WWNLI, KKKI, Z.

NLZI: This is the principal and orbital angular momentum quantum numbers (e.g. 1s→10).

XLI: This is the orbital angular momentum quantum number.

EEI: This is the eigenenergy of the orbital.

WWNLI: The occupation number (i.e. number of electrons) for the orbital.

KKKI: This is the number of points in the H-S mesh used to give the initial state radial wave function.

Z: This is the atomic number.

Data Card #3 (Format 19)

This card contains the 5 of the values of the initial radial wave function. There are (KKKI-1)/5+1 of these cards for the initial state radial wave function.

PIN(N): The values of the initial state radial wave function.

Data Card #4 (Format 21)

This card is the incident energy value (in threshold units) for which the ionization cross-section will be calculated.

c) Sample Output

The output from this program is a table of partial cross-sections Q equal the total cross-section Q obtained summing Q_λ . A sample output follows.

HELIUM**COUL-BORN

CROSS-SECTIONS ARE IN UNITS OF $\pi \cdot (\text{BOHR RADIUS})^2$.
 INCIDENT ENERGIES (N) ARE IN THRESHOLD ENERGY UNITS (EPSIL).
 EPSIL IS IN UNITS OF TWICE THE RYDBERG.

(AT. NO. = 1.) (EPSIL = 5.000E-01) (NL=N°L°:10-CONTINUUM)

L	I	SIG(L)	L	I	SIG(L)	L	I	SIG(L)
0.0	0	1.693E-01	1.000	0	6.615E-01	2.000	0	2.020E-01
3.000	0	3.678E-02	4.000	0	6.686E-03	5.000	0	1.256E-03

*N= 2.750 LOG(N)= 4.393E-01 SIG(TOTAL)= 1.078E 00

RHO(MAX)= 2.3229645E 01 ETA(MAX)=-9.7186023E-01

RHO(MIN)= 2.0704012E-04 ETA(MIN)=-1.0690455E 01

EXHIBIT 9

IONCST SAMPLE OUTPUT

TABLE A

Values for the starting potentials for the HFSWF program are given for each element. Also the occupation number and suggested eigenenergies for each orbital are listed.

0-17

U(X) X	HF 2	LI 3	BE 4	B 5	C 6	N 7	D 8	F 9
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	0.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.00000	0.99609	0.99529	0.99480	0.99432	0.99384	0.99337	0.99292
00.02	0.00000	0.99205	0.99041	0.98941	0.98845	0.98748	0.98653	0.98562
00.03	0.00000	0.98787	0.98539	0.98387	0.98241	0.98095	0.97952	0.97815
00.04	0.00000	0.98357	0.98023	0.97819	0.97624	0.97428	0.97238	0.97054
00.05	0.00000	0.97916	0.97495	0.97239	0.96995	0.96750	0.96513	0.96284
00.06	0.00000	0.97464	0.96957	0.96649	0.96356	0.96064	0.95781	0.95508
00.07	0.00000	0.97002	0.96409	0.96051	0.95711	0.95371	0.95043	0.94727
00.08	0.00000	0.96531	0.95853	0.95445	0.95059	0.94674	0.94302	0.93944
00.09	0.00000	0.96053	0.95290	0.94834	0.94403	0.93974	0.93560	0.93162
00.10	0.00000	0.95566	0.94721	0.94218	0.93745	0.93273	0.92818	0.92381
00.12	0.00000	0.94574	0.93568	0.92979	0.92424	0.91873	0.91341	0.90830
00.14	0.00000	0.93558	0.92402	0.91734	0.91107	0.90483	0.89880	0.89301
00.16	0.00000	0.92524	0.91228	0.90492	0.89800	0.89111	0.88443	0.87800
00.18	0.00000	0.91477	0.90053	0.89257	0.88509	0.87760	0.87033	0.86332
00.20	0.00000	0.90418	0.88880	0.88035	0.87238	0.86436	0.85654	0.84898
00.22	0.00000	0.89352	0.87713	0.86828	0.85991	0.85141	0.84308	0.83500
00.24	0.00000	0.88282	0.86555	0.85641	0.84769	0.83876	0.82996	0.82139
00.26	0.00000	0.87210	0.85410	0.84475	0.83574	0.82642	0.81718	0.80814
00.28	0.00000	0.86139	0.84279	0.83332	0.82408	0.81440	0.80474	0.79523
00.30	0.00000	0.85071	0.83165	0.82214	0.81271	0.80269	0.79263	0.78266
00.34	0.00000	0.82949	0.80992	0.80052	0.79083	0.78020	0.76934	0.75848
00.38	0.00000	0.80858	0.78899	0.77994	0.77007	0.75887	0.74722	0.73546
00.42	0.00000	0.78807	0.76892	0.76038	0.75038	0.73860	0.72614	0.71349
00.46	0.00000	0.76804	0.74972	0.74181	0.73168	0.71929	0.70601	0.69245
00.50	0.00000	0.74854	0.73140	0.72417	0.71389	0.70084	0.68671	0.67227
00.54	0.00000	0.72961	0.71392	0.70739	0.69690	0.68315	0.66817	0.65289
00.58	0.00000	0.71127	0.69727	0.69142	0.68065	0.66616	0.65033	0.63428
00.62	0.00000	0.69354	0.68140	0.67617	0.66506	0.64979	0.63316	0.61641
00.66	0.00000	0.67642	0.66628	0.66159	0.65005	0.63400	0.61661	0.59929
00.70	0.00000	0.65991	0.65195	0.64762	0.63557	0.61874	0.60069	0.58292
00.78	0.00000	0.62870	0.62491	0.62124	0.60802	0.58976	0.57073	0.55242
00.86	0.00000	0.59981	0.60021	0.59664	0.58213	0.56278	0.54333	0.52485
00.94	0.00000	0.57311	0.57740	0.57350	0.55777	0.53786	0.51849	0.49995
01.02	0.00000	0.54844	0.55620	0.55160	0.53493	0.51509	0.49609	0.47731
01.10	0.00000	0.52566	0.53636	0.53082	0.51367	0.49448	0.47585	0.45652
01.18	0.00000	0.50461	0.51766	0.51107	0.49409	0.47596	0.45741	0.43719
01.26	0.00000	0.50000	0.49995	0.49238	0.47628	0.45930	0.44042	0.41906
01.34	0.00000	0.50000	0.48309	0.47479	0.46026	0.44420	0.42458	0.40194
01.42	0.00000	0.50000	0.46699	0.45837	0.44596	0.43038	0.40965	0.38569
01.50	0.00000	0.50000	0.45159	0.44323	0.43319	0.41755	0.39549	0.37025
01.66	0.00000	0.50000	0.42277	0.41705	0.41136	0.39410	0.36908	0.34156
01.82	0.00000	0.50000	0.39654	0.39632	0.39294	0.37273	0.34486	0.31558
01.98	0.00000	0.50000	0.37307	0.38021	0.37659	0.35292	0.32259	0.29212
02.14	0.00000	0.50000	0.35267	0.36742	0.36151	0.33441	0.30215	0.27098
02.30	0.00000	0.50000	0.33560	0.35674	0.34730	0.31711	0.28341	0.25196
02.46	0.00000	0.50000	0.33333	0.34727	0.33379	0.30095	0.26628	0.23486
02.62	0.00000	0.50000	0.33333	0.33849	0.32089	0.28586	0.25061	0.21948
02.78	0.00000	0.50000	0.33333	0.33011	0.30857	0.27180	0.23629	0.20563
02.94	0.00000	0.50000	0.33333	0.32198	0.29681	0.25871	0.22319	0.19313
03.10	0.00000	0.50000	0.33333	0.31403	0.28559	0.24652	0.21120	0.18182
03.42	0.00000	0.50000	0.33333	0.29859	0.26478	0.22462	0.19011	0.16223
03.74	0.00000	0.50000	0.33333	0.28379	0.24597	0.20558	0.17224	0.14590
04.06	0.00000	0.50000	0.33333	0.26971	0.22902	0.18396	0.15696	0.13214
04.38	0.00000	0.50000	0.33333	0.25643	0.21375	0.17441	0.14380	0.12500
04.70	0.00000	0.50000	0.33333	0.25000	0.20001	0.16667	0.14286	0.12500
05.02	0.00000	0.50000	0.33333	0.25000	0.20000	0.16667	0.14286	0.12500

U(X) X	HE 2	LI 3	BE 4	B 5	C 6	N 7	O 8	F 9
05.34 0.00000	0.50000	0.33333	0.25000	0.20000	0.16667	0.14286	0.12500	0.11111
05.66 0.00000	0.50000	0.33333	0.25000	0.20000	0.16667	0.14286	0.12500	0.11111
05.98 0.00000	0.50000	0.33333	0.25000	0.20000	0.16667	0.14286	0.12500	0.11111
SHELL (1S) 0	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(-E) 0.	1.721	4.398	8.698	14.373	21.378	29.737	39.456	50.538
SHELL (2S) 0	(2S) 0	(2S) 1	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(-E) 0.	0.	.4039	.6012	0.9239	1.2895	1.6959	2.1440	2.6349
SHELL (2P) 0	(2P) 0	(2P) 0	(2P) 0	(2P) 1	(2P) 2	(2P) 3	(2P) 4	(2P) 5
(-E) 0.	0.	0.	0.	0.4898	0.6603	0.8445	1.0409	1.2502
U(X) X NE 10	NA 11	MG 12	AL 13	SI 14	P 15	S 16	CL 17	A 18
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00 1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01 0.99205	0.99186	0.99170	0.99157	0.99144	0.99131	0.99119	0.99106	0.99094
00.02 0.98387	0.98349	0.98317	0.98291	0.98265	0.98239	0.98213	0.98188	0.98164
00.03 0.97552	0.97496	0.97448	0.97408	0.97369	0.97330	0.97292	0.97255	0.97218
00.04 0.96705	0.96630	0.96567	0.96515	0.96463	0.96412	0.96363	0.96314	0.96266
00.05 0.95850	0.95758	0.95680	0.95616	0.95552	0.95490	0.95429	0.95370	0.95311
00.06 0.94990	0.94881	0.94790	0.94715	0.94641	0.94568	0.94497	0.94427	0.94359
00.07 0.94128	0.94003	0.93900	0.93815	0.93731	0.93649	0.93569	0.93490	0.93413
00.08 0.93266	0.93127	0.93012	0.92919	0.92827	0.92736	0.92648	0.92561	0.92475
00.09 0.92407	0.92255	0.92130	0.92029	0.91929	0.91831	0.91735	0.91641	0.91549
00.10 0.91553	0.91388	0.91254	0.91147	0.91041	0.90936	0.90834	0.90733	0.90634
00.12 0.89862	0.89677	0.89528	0.89411	0.89294	0.89179	0.89066	0.88954	0.88844
00.14 0.88202	0.88001	0.87841	0.87717	0.87593	0.87470	0.87348	0.87228	0.87109
00.16 0.86578	0.86364	0.86197	0.86069	0.85940	0.85811	0.85683	0.85556	0.85429
00.18 0.84994	0.84770	0.84598	0.84468	0.84335	0.84202	0.84069	0.83936	0.83802
00.20 0.83451	0.83219	0.83043	0.82913	0.82778	0.82642	0.82504	0.82366	0.82227
00.22 0.81947	0.81709	0.81532	0.81402	0.81266	0.81127	0.80987	0.80844	0.80700
00.24 0.80484	0.80241	0.80062	0.79934	0.79798	0.79657	0.79514	0.79368	0.79220
00.26 0.79058	0.78811	0.78632	0.78506	0.78370	0.78229	0.78083	0.77935	0.77785
00.28 0.77670	0.77419	0.77240	0.77117	0.76982	0.76840	0.76694	0.76545	0.76393
00.30 0.76316	0.76062	0.75884	0.75764	0.75631	0.75491	0.75345	0.75196	0.75044
00.34 0.73706	0.73447	0.73274	0.73164	0.73038	0.72904	0.72764	0.72620	0.72473
00.38 0.71215	0.70956	0.70791	0.70696	0.70584	0.70463	0.70335	0.70203	0.70066
00.42 0.68825	0.68580	0.68430	0.68357	0.68267	0.68165	0.68056	0.67940	0.67816
00.46 0.66558	0.66316	0.66187	0.66145	0.66083	0.66007	0.65920	0.65821	0.65710
00.50 0.64381	0.64160	0.64063	0.64058	0.64028	0.63980	0.63915	0.63832	0.63732
00.54 0.62303	0.62112	0.62053	0.62091	0.62096	0.62074	0.62028	0.61958	0.61866
00.58 0.60322	0.60170	0.60155	0.60236	0.60274	0.60276	0.60246	0.60186	0.60097
00.62 0.58438	0.58331	0.58360	0.58483	0.58551	0.58574	0.58556	0.58502	0.58416
00.66 0.56648	0.56589	0.56662	0.56823	0.56917	0.56955	0.56947	0.56899	0.56814
00.70 0.54948	0.54937	0.55050	0.55245	0.55361	0.55413	0.55413	0.55368	0.55285
00.78 0.51795	0.51868	0.52049	0.52300	0.52452	0.52527	0.52542	0.52506	0.52427
00.86 0.48923	0.49063	0.49296	0.49595	0.49779	0.49878	0.49910	0.49885	0.49813
00.94 0.46280	0.46473	0.46750	0.47096	0.47316	0.47442	0.47494	0.47483	0.47416
01.02 0.43822	0.44063	0.44387	0.44784	0.45043	0.45200	0.45274	0.45276	0.45214
01.10 0.41523	0.41815	0.42190	0.42643	0.42947	0.43137	0.43233	0.43246	0.43184
01.18 0.39363	0.39714	0.40148	0.40663	0.41014	0.41237	0.41353	0.41372	0.41304
01.26 0.37332	0.37752	0.38251	0.38833	0.39232	0.39486	0.39615	0.39634	0.39553
01.34 0.35422	0.35922	0.36492	0.37142	0.37587	0.37867	0.38004	0.38016	0.37916
01.42 0.33627	0.34216	0.34861	0.35578	0.36066	0.36366	0.36504	0.36502	0.36377
01.50 0.31941	0.32627	0.33349	0.34132	0.34657	0.34969	0.35102	0.35080	0.34927
01.66 0.28880	0.29777	0.30650	0.31549	0.32127	0.32444	0.32546	0.32473	0.32252
01.82 0.26198	0.27315	0.28323	0.29313	0.29915	0.30210	0.30266	0.30140	0.29887
01.98 0.23853	0.25186	0.26306	0.27356	0.27955	0.28212	0.28220	0.28058	0.27789
02.14 0.21805	0.23338	0.24541	0.25623	0.26199	0.26414	0.26389	0.26217	0.25953
02.30 0.20015	0.21726	0.22983	0.24074	0.24617	0.24799	0.24764	0.24603	0.24348
02.46 0.18447	0.20310	0.21594	0.22677	0.23189	0.23357	0.23335	0.23190	0.22926

U(X)	X	NE 10	NA 11	MG 12	AL 13	SI 14	P 15	S 16	CL 17	A 18
02.62	0.17068	0.19057	0.20345	0.21412	0.21905	0.22082	0.22083	0.21940	0.21645	
02.78	0.15851	0.17939	0.19215	0.20267	0.20758	0.20961	0.20980	0.20817	0.20468	
02.94	0.14773	0.16933	0.18188	0.19233	0.19743	0.19977	0.19995	0.19790	0.19376	
03.10	0.13812	0.16022	0.17251	0.18305	0.18849	0.19106	0.19102	0.18838	0.18354	
03.42	0.12180	0.14431	0.15626	0.16746	0.17369	0.17617	0.17509	0.17107	0.16493	
03.74	0.10847	0.13086	0.14301	0.15534	0.16187	0.16348	0.16102	0.15567	0.14852	
04.06	0.10000	0.11941	0.13248	0.14583	0.15193	0.15222	0.14837	0.14194	0.13412	
04.38	0.10000	0.10971	0.12425	0.13807	0.14314	0.14200	0.13695	0.12973	0.12152	
04.70	0.10000	0.10162	0.11781	0.13142	0.13516	0.13266	0.12664	0.11889	0.11053	
05.02	0.10000	0.09505	0.11263	0.12547	0.12779	0.12411	0.11736	0.10930	0.10094	
05.34	0.10000	0.09091	0.10829	0.11999	0.12094	0.11628	0.10901	0.10080	0.09255	
05.66	0.10000	0.09091	0.10449	0.11487	0.11457	0.10911	0.10148	0.09324	0.08517	
05.98	0.10000	0.09091	0.10105	0.11003	0.10864	0.10255	0.09470	0.08652	0.07866	
06.30	0.10000	0.09091	0.09784	0.10546	0.10311	0.09655	0.08858	0.08050	0.07289	
06.94	0.10000	0.09091	0.09191	0.09701	0.09317	0.08599	0.07799	0.07023	0.06311	
07.58	0.10000	0.09091	0.08646	0.08941	0.08454	0.07706	0.06921	0.06182	0.05556	
08.22	0.10000	0.09091	0.08333	0.08261	0.07704	0.06947	0.06250	0.05882	0.05556	
08.86	0.10000	0.09091	0.08333	0.07692	0.07143	0.06667	0.06250	0.05882	0.05556	
SHELL	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	
(-E)	62.99	78.05	94.95	113.66	134.04	156.11	179.89	205.36	232.54	
SHELL	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	
(-E)	2.168	4.723	6.552	8.715	11.087	13.684	16.510	19.570	22.865	
SHELL	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	
(-E)	1.471	2.669	4.144	5.947	7.954	10.180	12.628	15.303	18.207	
SHELL	(3S) 0	(3S) 1	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	
(-E)	0.	0.3777	0.5051	0.7445	0.9975	1.2588	1.5300	1.8124	2.1068	
SHELL	(3P) 0	(3P) 0	(3P) 0	(3P) 1	(3P) 2	(3P) 3	(3P) 4	(3P) 5	(3P) 6	
U(X)	X	K 19	CA 20	SC 21	TI 22	V 23	CR 24	MN 25	FE 26	CO 27
(-E)	0.	0.	0.	0.3582	0.4802	0.6139	0.7462	0.9067	1.0653	
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.99088	0.99082	0.99073	0.99064	0.99055	0.99043	0.99037	0.99027	0.99018	
00.02	0.98151	0.98140	0.98122	0.98104	0.98086	0.98063	0.98049	0.98030	0.98012	
00.03	0.97200	0.97184	0.97158	0.97131	0.97104	0.97069	0.97049	0.97021	0.96994	
00.04	0.96242	0.96221	0.96187	0.96152	0.96117	0.96071	0.96046	0.96009	0.95974	
00.05	0.95283	0.95258	0.95217	0.95175	0.95132	0.95076	0.95046	0.95002	0.94959	
00.06	0.94327	0.94299	0.94252	0.94203	0.94154	0.94089	0.94055	0.94003	0.93953	
00.07	0.93378	0.93348	0.93296	0.93241	0.93186	0.93112	0.93074	0.93016	0.92960	
00.08	0.92439	0.92408	0.92350	0.92291	0.92230	0.92148	0.92108	0.92043	0.91982	
00.09	0.91511	0.91479	0.91418	0.91354	0.91288	0.91199	0.91156	0.91086	0.91020	
00.10	0.90596	0.90564	0.90499	0.90431	0.90362	0.90265	0.90221	0.90146	0.90075	
00.12	0.88807	0.88777	0.88706	0.88632	0.88555	0.88446	0.88398	0.88314	0.88234	
00.14	0.87074	0.87048	0.86973	0.86894	0.86811	0.86690	0.86640	0.86548	0.86460	
00.16	0.85398	0.85377	0.85299	0.85215	0.85127	0.84994	0.84944	0.84844	0.84748	
00.18	0.83777	0.83761	0.83680	0.83593	0.83500	0.83357	0.83306	0.83199	0.83097	
00.20	0.82207	0.82197	0.82116	0.82025	0.81929	0.81775	0.81725	0.81611	0.81503	
00.22	0.80687	0.80685	0.80602	0.80509	0.80410	0.80247	0.80198	0.80079	0.79966	
00.24	0.79214	0.79220	0.79138	0.79044	0.78943	0.78771	0.78725	0.78601	0.78484	
00.26	0.77788	0.77803	0.77722	0.77628	0.77526	0.77347	0.77304	0.77177	0.77056	
00.28	0.76406	0.76432	0.76353	0.76261	0.76159	0.75974	0.75935	0.75805	0.75681	
00.30	0.75069	0.75107	0.75032	0.74942	0.74841	0.74650	0.74616	0.74483	0.74357	
00.34	0.72525	0.72592	0.72527	0.72444	0.72346	0.72144	0.72121	0.71983	0.71850	
00.38	0.70150	0.70249	0.70196	0.70120	0.70025	0.69811	0.69796	0.69650	0.69510	
00.42	0.67934	0.68064	0.68022	0.67951	0.67857	0.67626	0.67618	0.67462	0.67309	
00.46	0.65860	0.66019	0.65985	0.65916	0.65819	0.65570	0.65565	0.65396	0.65231	
00.50	0.63911	0.64096	0.64066	0.63996	0.63895	0.63625	0.63622	0.63439	0.63259	
00.54	0.62070	0.62280	0.62252	0.62179	0.62071	0.61778	0.61777	0.61579	0.61384	
00.58	0.60326	0.60557	0.60530	0.60453	0.60337	0.60022	0.60022	0.59809	0.59599	

U(X)	X	K	19	CA 20	SC 21	TI 22	V 23	CR 24	MN 25	FE 26	CO 27
00.62	0.58667	0.58920	0.58892	0.58811	0.58688	0.58350	0.58350	0.58123	0.57898		
00.66	0.57087	0.57361	0.57333	0.57247	0.57116	0.56755	0.56756	0.56513	0.56273		
00.70	0.55580	0.55875	0.55847	0.55756	0.55617	0.55232	0.55234	0.54976	0.54720		
00.78	0.52767	0.53105	0.53076	0.52975	0.52819	0.52385	0.52386	0.52096	0.51807		
00.86	0.50199	0.50578	0.50546	0.50432	0.50256	0.49771	0.49768	0.49443	0.49120		
00.94	0.47847	0.48265	0.48226	0.48095	0.47894	0.47355	0.47346	0.46985	0.46627		
01.02	0.45685	0.46137	0.46085	0.45933	0.45705	0.45109	0.45092	0.44696	0.44307		
01.10	0.43690	0.44169	0.44100	0.43922	0.43664	0.43013	0.42989	0.42562	0.42145		
01.18	0.41837	0.42337	0.42246	0.42041	0.41754	0.41051	0.41025	0.40571	0.40133		
01.26	0.40109	0.40624	0.40510	0.40279	0.39965	0.39216	0.39192	0.38719	0.38263		
01.34	0.38488	0.39016	0.38880	0.38626	0.38292	0.37502	0.37487	0.36998	0.36528		
01.42	0.36963	0.37504	0.37349	0.37078	0.36730	0.35905	0.35902	0.35399	0.34913		
01.50	0.35526	0.36082	0.35914	0.35633	0.35277	0.34420	0.34429	0.33910	0.33405		
01.66	0.32898	0.33502	0.33327	0.33040	0.32671	0.31744	0.31768	0.31207	0.30657		
01.82	0.30584	0.31261	0.31092	0.30794	0.30399	0.29387	0.29410	0.28796	0.28197		
01.98	0.28571	0.29324	0.29147	0.28819	0.28378	0.27269	0.27282	0.26617	0.25974		
02.14	0.26821	0.27632	0.27423	0.27043	0.26545	0.25341	0.25344	0.24637	0.23963		
02.30	0.25281	0.26122	0.25859	0.25420	0.24865	0.23576	0.23576	0.22839	0.22145		
02.46	0.23897	0.24744	0.24421	0.23923	0.23318	0.21957	0.21963	0.21208	0.20507		
02.62	0.22632	0.23471	0.23088	0.22539	0.21893	0.20476	0.20494	0.19733	0.19034		
02.78	0.21459	0.22286	0.21850	0.21258	0.20583	0.19124	0.19160	0.18401	0.17710		
02.94	0.20366	0.21181	0.20698	0.20074	0.19379	0.17891	0.17948	0.17198	0.16520		
03.10	0.19343	0.20148	0.19629	0.18981	0.18275	0.16768	0.16849	0.16111	0.15451		
03.42	0.17493	0.18287	0.17717	0.17043	0.16332	0.14817	0.14943	0.14240	0.13619		
03.74	0.15880	0.16667	0.16070	0.15391	0.14692	0.13199	0.13361	0.12698	0.12118		
04.06	0.14478	0.15257	0.14648	0.13977	0.13300	0.11848	0.12037	0.11415	0.10877		
04.38	0.13258	0.14022	0.13413	0.12759	0.12110	0.10712	0.10918	0.10338	0.09839		
04.70	0.12193	0.12934	0.12334	0.11703	0.11085	0.09750	0.09968	0.09427	0.08966		
05.02	0.11259	0.11969	0.11386	0.10783	0.10200	0.08929	0.09156	0.08653	0.08226		
05.34	0.10432	0.11110	0.10551	0.09981	0.09434	0.08225	0.08461	0.07993	0.07597		
05.66	0.09698	0.10346	0.09817	0.09283	0.08771	0.07618	0.07865	0.07429	0.07060		
05.98	0.09039	0.09667	0.09174	0.08676	0.08199	0.07094	0.07353	0.06945	0.06601		
06.30	0.08445	0.09067	0.08613	0.08151	0.07705	0.06639	0.06913	0.06528	0.06205		
06.94	0.07425	0.08087	0.07708	0.07305	0.06910	0.05897	0.06199	0.05853	0.05562		
07.58	0.06596	0.07359	0.07034	0.06669	0.06306	0.05327	0.05649	0.05330	0.05061		
08.22	0.05937	0.06822	0.06521	0.06174	0.05829	0.04880	0.05208	0.04909	0.04657		
08.86	0.05431	0.06413	0.06113	0.05772	0.05436	0.04521	0.04841	0.04558	0.04321		
09.50	0.05263	0.06083	0.05771	0.05430	0.05101	0.04226	0.04527	0.04258	0.04032		
10.14	0.05263	0.05798	0.05471	0.05129	0.04805	0.04167	0.04252	0.03995	0.03781		
10.78	0.05263	0.05543	0.05201	0.04858	0.04541	0.04167	0.04008	0.03846	0.03704		
11.42	0.05263	0.05306	0.04953	0.04611	0.04348	0.04167	0.04000	0.03846	0.03704		
12.06	0.05263	0.05085	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
12.70	0.05263	0.05000	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
13.98	0.05263	0.05000	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
15.26	0.05263	0.05000	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
16.54	0.05263	0.05000	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
17.82	0.05263	0.05000	0.04762	0.04545	0.04348	0.04167	0.04000	0.03846	0.03704		
SHELL	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2		
(=E)	262.09	293.52	326.29	360.77	396.95	434.45	474.47	515.81	558.89		
SHELL	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2		
(=E)	27.060	31.627	35.973	40.521	45.289	49.823	55.509	60.957	66.648		
SHELL	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6		
(=E)	22.008	26.180	30.130	34.279	38.646	42.779	48.050	53.084	58.358		
SHELL	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2		
(=E)	2.9521	3.8750	4.4308	4.9813	5.5371	5.7114	6.6804	7.2691	7.8785		
SHELL	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6		
(=E)	1.7328	2.4823	2.8831	3.2760	3.6704	3.6910	4.4776	4.8912	5.3200		
SHELL	(3D) 0	(3D) 0	(3D) 1	(3D) 2	(3D) 3	(3D) 4	(3D) 5	(3D) 6	(3D) 7		

(-E)	0.	0.	0.5308	0.6279	0.7183	0.4789	0.8859	0.9625	1.0415
SHELL	(4S) 1	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 1	(4S) 2	(4S) 2	(4S) 2
(-E)	0.3086	0.3987	0.4309	0.4578	0.4819	0.4312	0.5253	0.5451	0.5647
U(X) X	NI 28	CU 29	ZN 30	GA 31	GE 32	AS 33	SE 34	BR 35	KR 36
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.99009	0.98997	0.98990	0.98984	0.98979	0.98973	0.98968	0.98963	0.98958
00.02	0.97993	0.97969	0.97956	0.97945	0.97933	0.97923	0.97912	0.97902	0.97892
00.03	0.96966	0.96931	0.96912	0.96895	0.96879	0.96863	0.96848	0.96833	0.96819
00.04	0.95938	0.95892	0.95867	0.95846	0.95825	0.95805	0.95786	0.95767	0.95748
00.05	0.94915	0.94859	0.94829	0.94803	0.94779	0.94755	0.94732	0.94710	0.94688
00.06	0.93903	0.93837	0.93802	0.93773	0.93745	0.93719	0.93693	0.93667	0.93642
00.07	0.92903	0.92828	0.92789	0.92758	0.92727	0.92698	0.92669	0.92641	0.92614
00.08	0.91919	0.91835	0.91793	0.91759	0.91726	0.91695	0.91664	0.91634	0.91604
00.09	0.90951	0.90859	0.90814	0.90778	0.90743	0.90710	0.90677	0.90645	0.90613
00.10	0.90001	0.89901	0.89853	0.89815	0.89778	0.89743	0.89709	0.89675	0.89642
00.12	0.88151	0.88036	0.87983	0.87943	0.87903	0.87865	0.87828	0.87792	0.87756
00.14	0.86367	0.86238	0.86182	0.86139	0.86096	0.86057	0.86018	0.85979	0.85941
00.16	0.84648	0.84504	0.84445	0.84400	0.84356	0.84315	0.84274	0.84235	0.84195
00.18	0.82988	0.82832	0.82769	0.82724	0.82679	0.82638	0.82596	0.82556	0.82516
00.20	0.81388	0.81218	0.81154	0.81108	0.81063	0.81023	0.80981	0.80941	0.80902
00.22	0.79844	0.79663	0.79598	0.79553	0.79509	0.79469	0.79429	0.79390	0.79352
00.24	0.78357	0.78165	0.78099	0.78056	0.78013	0.77975	0.77937	0.77899	0.77862
00.26	0.76925	0.76722	0.76657	0.76615	0.76575	0.76538	0.76502	0.76466	0.76430
00.28	0.75546	0.75333	0.75268	0.75229	0.75190	0.75156	0.75120	0.75085	0.75051
00.30	0.74218	0.73994	0.73930	0.73892	0.73855	0.73822	0.73788	0.73754	0.73719
00.34	0.71702	0.71456	0.71390	0.71355	0.71319	0.71287	0.71253	0.71219	0.71184
00.38	0.69350	0.69077	0.69009	0.68973	0.68936	0.68903	0.68868	0.68833	0.68796
00.42	0.67135	0.66835	0.66761	0.66724	0.66685	0.66650	0.66613	0.66575	0.66536
00.46	0.65040	0.64711	0.64631	0.64591	0.64549	0.64513	0.64473	0.64434	0.64393
00.50	0.63052	0.62693	0.62607	0.62564	0.62520	0.62481	0.62439	0.62398	0.62355
00.54	0.61161	0.60771	0.60679	0.60633	0.60587	0.60546	0.60503	0.60459	0.60415
00.58	0.59359	0.58939	0.58840	0.58792	0.58743	0.58701	0.58656	0.58611	0.58564
00.62	0.57640	0.57189	0.57085	0.57034	0.56983	0.56939	0.56892	0.56845	0.56796
00.66	0.55998	0.55517	0.55406	0.55352	0.55299	0.55253	0.55204	0.55155	0.55105
00.70	0.54427	0.53915	0.53797	0.53742	0.53686	0.53637	0.53587	0.53537	0.53486
00.78	0.51478	0.50905	0.50773	0.50712	0.50652	0.50600	0.50548	0.50497	0.50445
00.86	0.48754	0.48120	0.47976	0.47911	0.47848	0.47797	0.47745	0.47697	0.47648
00.94	0.46226	0.45534	0.45380	0.45315	0.45255	0.45207	0.45161	0.45120	0.45078
01.02	0.43874	0.43128	0.42969	0.42909	0.42856	0.42818	0.42781	0.42749	0.42717
01.10	0.41686	0.40892	0.40733	0.40683	0.40640	0.40612	0.40586	0.40564	0.40540
01.18	0.39653	0.38816	0.38660	0.38621	0.38590	0.38573	0.38556	0.38542	0.38525
01.26	0.37765	0.36888	0.36736	0.36708	0.36687	0.36678	0.36669	0.36662	0.36651
01.34	0.36013	0.35093	0.34944	0.34926	0.34913	0.34911	0.34909	0.34908	0.34902
01.42	0.34379	0.33416	0.33267	0.33257	0.33251	0.33257	0.33261	0.33266	0.33266
01.50	0.32850	0.31841	0.31692	0.31689	0.31691	0.31703	0.31715	0.31728	0.31736
01.66	0.30054	0.28955	0.28805	0.28819	0.28840	0.28872	0.28905	0.28939	0.28967
01.82	0.27547	0.26368	0.26225	0.26265	0.26314	0.26374	0.26434	0.26495	0.26547
01.98	0.25289	0.24044	0.23919	0.23996	0.24081	0.24176	0.24268	0.24356	0.24431
02.14	0.23254	0.21962	0.21864	0.21936	0.22113	0.22245	0.22369	0.22483	0.22577
02.30	0.21427	0.20102	0.20039	0.20211	0.20382	0.20549	0.20702	0.20836	0.20943
02.46	0.19789	0.18445	0.18422	0.18644	0.18857	0.19057	0.19232	0.19380	0.19492
02.62	0.18325	0.16972	0.16990	0.17262	0.17513	0.17739	0.17930	0.18085	0.18195
02.78	0.17015	0.15664	0.15721	0.16039	0.16323	0.16568	0.16769	0.16924	0.17029
02.94	0.15844	0.14501	0.14596	0.14955	0.15265	0.15524	0.15728	0.15879	0.15976
03.10	0.14795	0.13467	0.13595	0.13989	0.14320	0.14586	0.14790	0.14934	0.15022
03.42	0.13008	0.11722	0.11904	0.12354	0.12709	0.12977	0.13171	0.13301	0.13376
03.74	0.11552	0.10322	0.10541	0.11027	0.11390	0.11652	0.11835	0.11956	0.12024

U(X) X	NI 28	CU 29	ZN 30	GA 31	GE 32	AS 33	SE 34	BR 35	KR 36
04.06	0.10355	0.09185	0.09427	0.09936	0.10299	0.10553	0.10730	0.10845	0.10906
04.38	0.09358	0.08251	0.08507	0.09030	0.09390	0.09639	0.09812	0.09920	0.09965
04.70	0.08521	0.07475	0.07740	0.08272	0.08630	0.08876	0.09042	0.09135	0.09154
05.02	0.07815	0.06825	0.07095	0.07634	0.07991	0.08232	0.08385	0.08454	0.08441
05.34	0.07217	0.06276	0.06551	0.07095	0.07449	0.07681	0.07813	0.07852	0.07807
05.66	0.06707	0.05807	0.06088	0.06636	0.06985	0.07201	0.07308	0.07315	0.07238
05.98	0.06270	0.05406	0.05692	0.06241	0.06581	0.06776	0.06855	0.06831	0.06725
06.30	0.05894	0.05058	0.05350	0.05898	0.06224	0.06396	0.06445	0.06392	0.06263
06.94	0.05282	0.04492	0.04792	0.05328	0.05619	0.05738	0.05732	0.05631	0.05466
07.58	0.04804	0.04052	0.04355	0.04867	0.05116	0.05185	0.05132	0.04997	0.04811
08.22	0.04418	0.03703	0.04001	0.04482	0.04687	0.04711	0.04623	0.04465	0.04268
08.86	0.04095	0.03448	0.03706	0.04151	0.04314	0.04302	0.04187	0.04014	0.03811
09.50	0.03820	0.03448	0.03454	0.03861	0.03988	0.03945	0.03811	0.03628	0.03424
10.14	0.03580	0.03448	0.03333	0.03605	0.03699	0.03632	0.03483	0.03294	0.03092
10.78	0.03571	0.03448	0.03333	0.03376	0.03442	0.03356	0.03196	0.03004	0.02805
11.42	0.03571	0.03448	0.03333	0.03226	0.03214	0.03111	0.02944	0.02857	0.02778
12.06	0.03571	0.03448	0.03333	0.03226	0.03125	0.03030	0.02941	0.02857	0.02778
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(=E) 603.7	649.7	698.4	749.2	801.8	856.3	912.5	970.7	1030.6	
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(=E) 72.57	78.15	85.12	92.64	100.51	108.73	117.30	126.24	135.53	
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(=E) 63.86	69.02	75.55	82.63	90.05	97.82	105.95	114.43	123.25	
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(=E) 8.500	8.634	9.793	11.238	12.762	14.375	16.074	17.857	19.728	
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(=E) 5.756	5.709	6.661	7.892	9.197	10.587	12.058	13.611	15.249	
SHELL (3D) 8	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(=E) 1.1151	0.7431	1.2582	2.0400	2.8901	3.8229	4.8340	5.9245	7.0975	
SHELL (4S) 2	(4S) 1	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(=E) 0.5831	0.5091	0.6185	0.8377	1.0571	1.2754	1.4953	1.7185	1.9456	
SHELL (4P) 0	(4P) 0	(4P) 0	(4P) 1	(4P) 1	(4P) 2	(4P) 3	(4P) 4	(4P) 5	(4P) 6
(=E) 0.	0.	0.	0.3619	0.4683	0.5826	0.7015	0.8247	0.9519	
U(X) X	RB 37	SR 38	YT 39	ZR 40	NB 41	MD 42	TC 43	RU 44	RH 45
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.98955	0.98952	0.98948	0.98944	0.98940	0.98936	0.98933	0.98928	0.98924
00.02	0.97886	0.97880	0.97873	0.97866	0.97857	0.97849	0.97844	0.97834	0.97827
00.03	0.96810	0.96802	0.96792	0.96781	0.96768	0.96757	0.96749	0.96736	0.96725
00.04	0.95738	0.95728	0.95715	0.95702	0.95685	0.95672	0.95661	0.95644	0.95630
00.05	0.94676	0.94665	0.94650	0.94635	0.94615	0.94599	0.94588	0.94567	0.94551
00.06	0.93625	0.93617	0.93601	0.93584	0.93562	0.93544	0.93531	0.93508	0.93490
00.07	0.92600	0.92588	0.92570	0.92552	0.92528	0.92509	0.92495	0.92469	0.92450
00.08	0.91590	0.91578	0.91560	0.91540	0.91514	0.91494	0.91480	0.91452	0.91430
00.09	0.90600	0.90588	0.90569	0.90549	0.90521	0.90499	0.90485	0.90455	0.90433
00.10	0.89629	0.89617	0.89598	0.89577	0.89548	0.89525	0.89511	0.89479	0.89455
00.12	0.87744	0.87734	0.87714	0.87692	0.87660	0.87636	0.87623	0.87587	0.87562
00.14	0.85931	0.85923	0.85903	0.85882	0.85848	0.85823	0.85811	0.85772	0.85745
00.16	0.84188	0.84182	0.84164	0.84143	0.84107	0.84083	0.84072	0.84031	0.84004
00.18	0.82512	0.82510	0.82493	0.82474	0.82437	0.82413	0.82405	0.82362	0.82335
00.20	0.80902	0.80905	0.80890	0.80872	0.80836	0.80814	0.80808	0.80764	0.80738
00.22	0.79356	0.79364	0.79352	0.79337	0.79301	0.79280	0.79277	0.79232	0.79206
00.24	0.77872	0.77884	0.77875	0.77863	0.77827	0.77807	0.77807	0.77760	0.77735
00.26	0.76444	0.76462	0.76456	0.76445	0.76408	0.76389	0.76392	0.76344	0.76317
00.28	0.75070	0.75091	0.75087	0.75078	0.75041	0.75022	0.75027	0.74976	0.74949
00.30	0.73742	0.73768	0.73766	0.73757	0.73719	0.73700	0.73706	0.73653	0.73625
00.34	0.71214	0.71246	0.71246	0.71238	0.71196	0.71177	0.71186	0.71126	0.71095
00.38	0.68831	0.68869	0.68870	0.68863	0.68817	0.68797	0.68808	0.68742	0.68709

U(X)	X	RB 37	SR 38	YT 39	ZR 40	NR 41	MC 42	TC 43	RU 44	RF 45
00.42	0.66577	0.66620	0.66623	0.66616	0.66566	0.66545	0.66558	0.66486	0.66451	
00.46	0.64438	0.64487	0.64491	0.64486	0.64432	0.64409	0.64426	0.64348	0.64310	
00.50	0.62406	0.62461	0.62467	0.62462	0.62405	0.62381	0.62401	0.62317	0.62278	
00.54	0.60471	0.60532	0.60540	0.60536	0.60475	0.60451	0.60474	0.60385	0.60345	
00.58	0.58626	0.58693	0.58703	0.58700	0.58637	0.58612	0.58638	0.58545	0.58503	
00.62	0.56864	0.56938	0.56949	0.56948	0.56882	0.56858	0.56888	0.56791	0.56749	
00.66	0.55179	0.55259	0.55273	0.55274	0.55206	0.55183	0.55218	0.55117	0.55076	
00.70	0.53566	0.53652	0.53670	0.53673	0.53604	0.53584	0.53624	0.53522	0.53482	
00.78	0.50540	0.50643	0.50670	0.50681	0.50613	0.50600	0.50654	0.50550	0.50516	
00.86	0.47762	0.47886	0.47926	0.47949	0.47885	0.47881	0.47951	0.47846	0.47818	
00.94	0.45215	0.45362	0.45417	0.45453	0.45394	0.45398	0.45483	0.45377	0.45353	
01.02	0.42877	0.43046	0.43116	0.43164	0.43108	0.43119	0.43218	0.43109	0.43088	
01.10	0.40723	0.40914	0.40997	0.41055	0.41000	0.41018	0.41129	0.41016	0.40998	
01.18	0.38728	0.38939	0.39034	0.39102	0.39048	0.39072	0.39195	0.39079	0.39065	
01.26	0.36874	0.37104	0.37211	0.37288	0.37236	0.37266	0.37403	0.37284	0.37273	
01.34	0.35144	0.35395	0.35514	0.35602	0.35552	0.35590	0.35740	0.35619	0.35611	
01.42	0.33530	0.33802	0.33934	0.34033	0.33987	0.34033	0.34196	0.34072	0.34068	
01.50	0.32022	0.32316	0.32463	0.32574	0.32532	0.32585	0.32761	0.32634	0.32632	
01.66	0.29301	0.29642	0.29819	0.29954	0.29918	0.29984	0.30182	0.30044	0.30041	
01.82	0.26930	0.27318	0.27523	0.27678	0.27642	0.27715	0.27928	0.27771	0.27759	
01.98	0.24862	0.25292	0.25518	0.25687	0.25645	0.25715	0.25937	0.25754	0.25727	
02.14	0.23049	0.23514	0.23755	0.23930	0.23872	0.23935	0.24160	0.23947	0.23904	
02.30	0.21449	0.21942	0.22190	0.22364	0.22287	0.22339	0.22566	0.22324	0.22266	
02.46	0.20026	0.20540	0.20792	0.20962	0.20863	0.20903	0.21135	0.20866	0.20798	
02.62	0.18752	0.19285	0.19536	0.19701	0.19580	0.19613	0.19852	0.19559	0.19482	
02.78	0.17605	0.18155	0.18407	0.18568	0.18428	0.18454	0.18702	0.18384	0.18297	
02.94	0.16570	0.17139	0.17392	0.17551	0.17393	0.17412	0.17667	0.17323	0.17221	
03.10	0.15637	0.16225	0.16480	0.16638	0.16460	0.16471	0.16728	0.16353	0.16232	
03.42	0.14035	0.14665	0.14921	0.15068	0.14844	0.14825	0.15073	0.14629	0.14464	
03.74	0.12729	0.13390	0.13633	0.13754	0.13471	0.13411	0.13639	0.13129	0.12923	
04.06	0.11645	0.12320	0.12535	0.12619	0.12273	0.12171	0.12379	0.11811	0.11574	
04.38	0.10722	0.11396	0.11575	0.11617	0.11213	0.11073	0.11265	0.10655	0.10398	
04.70	0.09918	0.10581	0.10721	0.10724	0.10271	0.10102	0.10282	0.09643	0.09376	
05.02	0.09206	0.09853	0.09957	0.09925	0.09434	0.09242	0.09414	0.08759	0.08488	
05.34	0.08570	0.09199	0.09269	0.09208	0.08688	0.08482	0.08648	0.07987	0.07718	
05.66	0.07998	0.08608	0.08648	0.08563	0.08025	0.07810	0.07971	0.07312	0.07049	
05.98	0.07482	0.08073	0.08086	0.07982	0.07435	0.07215	0.07371	0.06721	0.06466	
06.30	0.07017	0.07585	0.07577	0.07458	0.06908	0.06687	0.06839	0.06202	0.05957	
06.94	0.06211	0.06732	0.06692	0.06557	0.06017	0.05800	0.05946	0.05343	0.05118	
07.58	0.05540	0.06015	0.05957	0.05819	0.05300	0.05094	0.05236	0.04670	0.04464	
08.22	0.04972	0.05408	0.05349	0.05216	0.04720	0.04527	0.04669	0.04134	0.03946	
08.86	0.04487	0.04899	0.04848	0.04726	0.04248	0.04067	0.04213	0.03703	0.03530	
09.50	0.04070	0.04477	0.04440	0.04327	0.03862	0.03692	0.03843	0.03352	0.03192	
10.14	0.03710	0.04132	0.04108	0.04001	0.03543	0.03382	0.03537	0.03063	0.02914	
10.78	0.03402	0.03855	0.03838	0.03732	0.03278	0.03124	0.03282	0.02821	0.02681	
11.42	0.03142	0.03631	0.03614	0.03505	0.03054	0.02906	0.03064	0.02617	0.02486	
12.06	0.02926	0.03449	0.03424	0.03309	0.02863	0.02719	0.02875	0.02443	0.02319	
12.70	0.02750	0.03296	0.03258	0.03138	0.02698	0.02558	0.02708	0.02293	0.02222	
13.98	0.02703	0.03047	0.02978	0.02844	0.02439	0.02381	0.02427	0.02273	0.02222	
15.26	0.02703	0.02840	0.02742	0.02598	0.02439	0.02381	0.02326	0.02273	0.02222	
16.54	0.02703	0.02657	0.02564	0.02500	0.02439	0.02381	0.02326	0.02273	0.02222	
17.82	0.02703	0.02632	0.02564	0.02500	0.02439	0.02381	0.02326	0.02273	0.02222	
SHELL	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	
(=E)	1092.9	1157.2	1223.0	1290.7	1359.9	1431.2	1504.6	1579.2	1656.0	
SHELL	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	
(=E)	145.68	156.27	166.97	177.97	189.03	200.68	212.98	224.97	237.63	
SHELL	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	
(=E)	132.94	143.06	153.29	163.83	174.41	185.58	197.41	208.92	221.09	

U(X) X	RB 37	SR 38	YT 39	ZR 40	NB 41	MC 42	TC 43	RU 44	RF 45
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(-E) 22.203	24.820	27.285	29.797	32.100	34.711	37.720	40.156	42.990	
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(-E) 17.487	19.866	22.089	24.358	26.415	28.780	31.539	33.725	36.305	
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(-E) 8.869	10.777	12.528	14.322	15.901	17.785	20.063	21.761	23.853	
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(-E) 2.6124	3.3055	3.7821	4.2339	4.4359	4.8484	5.5469	5.6733	6.0877	
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(-E) 1.4775	2.0351	2.3929	2.7285	2.8271	3.1252	3.6974	3.7207	4.0197	
SHELL (4D) 0	(4D) 0	(4D) 1	(4D) 2	(4D) 4	(4D) 5	(4D) 5	(4D) 7	(4D) 8	
(-E) 0.	0.	0.4088	0.5159	0.4478	0.5261	0.8259	0.6857	0.7663	
SHELL (5S) 1	(5S) 2	(5S) 2	(5S) 2	(5S) 1	(5S) 1	(5S) 2	(5S) 1	(5S) 1	
(-E) 0.2905	0.3682	0.4069	0.4359	0.4019	0.4169	0.4980	0.4424	0.4533	
U(X) X	PD 46	AG 47	CD 48	IN 49	SN 50	SR 51	TE 52	I 53	XE 54
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.98920	0.98917	0.98914	0.98911	0.98909	0.98907	0.98904	0.98902	0.98900
00.02	0.97817	0.97811	0.97806	0.97801	0.97797	0.97792	0.97788	0.97783	0.97779
00.03	0.96711	0.96703	0.96695	0.96689	0.96682	0.96676	0.96670	0.96664	0.96658
00.04	0.95612	0.95603	0.95593	0.95586	0.95578	0.95570	0.95563	0.95556	0.95549
00.05	0.94530	0.94519	0.94508	0.94499	0.94490	0.94482	0.94474	0.94465	0.94457
00.06	0.93466	0.93454	0.93442	0.93432	0.93423	0.93414	0.93405	0.93397	0.93388
00.07	0.92423	0.92410	0.92397	0.92388	0.92378	0.92369	0.92360	0.92351	0.92342
00.08	0.91402	0.91388	0.91375	0.91365	0.91355	0.91346	0.91336	0.91327	0.91319
00.09	0.90402	0.90387	0.90374	0.90364	0.90354	0.90345	0.90336	0.90327	0.90318
00.10	0.89423	0.89408	0.89394	0.89385	0.89375	0.89366	0.89357	0.89348	0.89339
00.12	0.87525	0.87510	0.87496	0.87488	0.87479	0.87470	0.87462	0.87454	0.87446
00.14	0.85705	0.85691	0.85678	0.85671	0.85663	0.85656	0.85649	0.85643	0.85636
00.16	0.83961	0.83948	0.83936	0.83931	0.83926	0.83921	0.83916	0.83911	0.83907
00.18	0.82291	0.82279	0.82270	0.82267	0.82264	0.82262	0.82259	0.82257	0.82254
00.20	0.80692	0.80682	0.80674	0.80674	0.80674	0.80674	0.80674	0.80674	0.80674
00.22	0.79158	0.79150	0.79145	0.79147	0.79149	0.79151	0.79153	0.79155	0.79157
00.24	0.77685	0.77678	0.77674	0.77679	0.77683	0.77687	0.77690	0.77694	0.77697
00.26	0.76265	0.76259	0.76256	0.76263	0.76269	0.76274	0.76279	0.76284	0.76288
00.28	0.74894	0.74888	0.74887	0.74895	0.74901	0.74908	0.74914	0.74920	0.74926
00.30	0.73566	0.73561	0.73560	0.73569	0.73577	0.73585	0.73592	0.73600	0.73606
00.34	0.71030	0.71026	0.71025	0.71037	0.71047	0.71057	0.71067	0.71076	0.71084
00.38	0.68637	0.68633	0.68633	0.68648	0.68661	0.68673	0.68685	0.68697	0.68708
00.42	0.66372	0.66369	0.66371	0.66389	0.66404	0.66419	0.66434	0.66449	0.66462
00.46	0.64226	0.64224	0.64228	0.64248	0.64267	0.64285	0.64303	0.64321	0.64338
00.50	0.62187	0.62187	0.62193	0.62217	0.62239	0.62261	0.62282	0.62304	0.62325
00.54	0.60248	0.60250	0.60258	0.60287	0.60313	0.60339	0.60365	0.60391	0.60416
00.58	0.58402	0.58406	0.58418	0.58451	0.58483	0.58514	0.58544	0.58576	0.58605
00.62	0.56643	0.56651	0.56667	0.56706	0.56743	0.56779	0.56816	0.56853	0.56889
00.66	0.54968	0.54979	0.55000	0.55046	0.55089	0.55132	0.55175	0.55219	0.55261
00.70	0.53372	0.53388	0.53415	0.53468	0.53518	0.53568	0.53617	0.53667	0.53715
00.78	0.50402	0.50430	0.50469	0.50537	0.50601	0.50665	0.50727	0.50789	0.50849
00.86	0.47702	0.47741	0.47791	0.47873	0.47950	0.48025	0.48100	0.48173	0.48243
00.94	0.45233	0.45282	0.45342	0.45436	0.45525	0.45612	0.45696	0.45779	0.45858
01.02	0.42962	0.43021	0.43091	0.43196	0.43296	0.43393	0.43488	0.43580	0.43668
01.10	0.40868	0.40934	0.41013	0.41131	0.41241	0.41349	0.41453	0.41554	0.41650
01.18	0.38930	0.39004	0.39093	0.39222	0.39343	0.39460	0.39573	0.39682	0.39786
01.26	0.37133	0.37217	0.37314	0.37454	0.37585	0.37711	0.37831	0.37947	0.38056
01.34	0.35466	0.35558	0.35663	0.35813	0.35953	0.36086	0.36212	0.36333	0.36446
01.42	0.33917	0.34016	0.34128	0.34286	0.34432	0.34570	0.34701	0.34825	0.34940
01.50	0.32474	0.32578	0.32695	0.32859	0.33010	0.33152	0.33285	0.33410	0.33526
01.66	0.29862	0.29971	0.30092	0.30265	0.30420	0.30565	0.30700	0.30826	0.30942

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U(X)	X	PD 46	AG 47	CD 48	IN 49	SN 50	SR 51	TF 52	I 53	XE 54
01.82	0.27552	0.27661	0.27780	0.27956	0.28115	0.28262	0.28399	0.28529	0.28650	0.28650
01.98	0.25489	0.25593	0.25711	0.25892	0.26056	0.26210	0.26355	0.26493	0.26623	0.26623
02.14	0.23634	0.23737	0.23858	0.24049	0.24223	0.24387	0.24543	0.24690	0.24827	0.24827
02.30	0.21968	0.22074	0.22202	0.22405	0.22591	0.22765	0.22927	0.23078	0.23216	0.23216
02.46	0.20475	0.20586	0.20720	0.20935	0.21128	0.21305	0.21469	0.21618	0.21753	0.21753
02.62	0.19133	0.19248	0.19385	0.19605	0.19800	0.19977	0.20137	0.20281	0.20409	0.20409
02.78	0.17920	0.18033	0.18168	0.18389	0.18582	0.18755	0.18910	0.19048	0.19170	0.19170
02.94	0.16810	0.16918	0.17047	0.17267	0.17456	0.17625	0.17776	0.17909	0.18026	0.18026
03.10	0.15787	0.15886	0.16008	0.16226	0.16414	0.16579	0.16727	0.16857	0.16970	0.16970
03.42	0.13948	0.14032	0.14144	0.14364	0.14552	0.14717	0.14864	0.14990	0.15099	0.15099
03.74	0.12345	0.12423	0.12532	0.12763	0.12958	0.13129	0.13277	0.13402	0.13506	0.13506
04.06	0.10950	0.11031	0.11146	0.11393	0.11600	0.11777	0.11926	0.12047	0.12144	0.12144
04.38	0.09741	0.09833	0.09960	0.10225	0.10442	0.10623	0.10771	0.10884	0.10972	0.10972
04.70	0.08699	0.08807	0.08945	0.09228	0.09453	0.09635	0.09777	0.09882	0.09959	0.09959
05.02	0.07803	0.07927	0.08077	0.08374	0.08604	0.08783	0.08918	0.09014	0.09082	0.09082
05.34	0.07032	0.07173	0.07331	0.07640	0.07871	0.08045	0.08173	0.08261	0.08324	0.08324
05.66	0.06369	0.06525	0.06690	0.07006	0.07235	0.07404	0.07526	0.07609	0.07669	0.07669
05.98	0.05796	0.05965	0.06134	0.06455	0.06682	0.06845	0.06963	0.07043	0.07100	0.07100
06.30	0.05301	0.05480	0.05651	0.05975	0.06198	0.06358	0.06473	0.06550	0.06604	0.06604
06.94	0.04495	0.04688	0.04861	0.05187	0.05405	0.05559	0.05670	0.05737	0.05775	0.05775
07.58	0.03876	0.04077	0.04249	0.04576	0.04790	0.04941	0.05041	0.05091	0.05106	0.05106
08.22	0.03392	0.03595	0.03770	0.04097	0.04308	0.04449	0.04533	0.04560	0.04548	0.04548
08.86	0.03006	0.03211	0.03389	0.03715	0.03919	0.04046	0.04109	0.04112	0.04077	0.04077
09.50	0.02693	0.02898	0.03082	0.03405	0.03598	0.03707	0.03747	0.03728	0.03675	0.03675
10.14	0.02434	0.02642	0.02830	0.03147	0.03327	0.03416	0.03434	0.03396	0.03328	0.03328
10.78	0.02218	0.02429	0.02620	0.02928	0.03092	0.03161	0.03160	0.03107	0.03028	0.03028
11.42	0.02174	0.02251	0.02442	0.02738	0.02886	0.02936	0.02919	0.02853	0.02766	0.02766
12.06	0.02174	0.02128	0.02289	0.02571	0.02702	0.02735	0.02703	0.02628	0.02535	0.02535
12.70	0.02174	0.02128	0.02155	0.02423	0.02537	0.02555	0.02511	0.02427	0.02331	0.02331
13.98	0.02174	0.02128	0.02083	0.02169	0.02253	0.02244	0.02182	0.02087	0.01987	0.01987
15.26	0.02174	0.02128	0.02083	0.02041	0.02017	0.01987	0.01923	0.01887	0.01852	0.01852
16.54	0.02174	0.02128	0.02083	0.02041	0.02000	0.01961	0.01923	0.01887	0.01852	0.01852
17.82	0.02174	0.02128	0.02083	0.02041	0.02000	0.01961	0.01923	0.01887	0.01852	0.01852
SHELL	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(-E)	1734.3	1815.0	1897.7	1982.5	2069.1	2157.6	2248.0	2340.3	2434.4	2434.4
SHELL	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(-E)	250.28	263.96	278.08	292.76	307.82	323.27	339.13	355.39	372.05	372.05
SHELL	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(-E)	233.26	246.45	260.08	274.27	288.83	303.78	319.14	334.90	351.05	351.05
SHELL	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(-E)	45.558	48.886	52.393	56.173	60.068	64.091	68.245	72.529	76.945	76.945
SHELL	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(-E)	38.619	41.691	44.940	48.459	52.093	55.853	59.743	63.761	67.910	67.910
SHELL	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(-E)	25.674	28.253	31.005	34.025	37.159	40.417	43.802	47.314	50.955	50.955
SHELL	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(-E)	6.185	6.925	7.745	8.743	9.761	10.812	11.899	13.023	14.184	14.184
SHELL	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(-E)	4.009	4.624	5.313	6.178	7.060	7.973	8.921	9.903	10.923	10.923
SHELL	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(-E)	0.5861	0.9300	1.3439	1.9269	2.5262	3.1564	3.8208	4.5206	5.2570	5.2570
SHELL	(5S) 0	(5S) 1	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(-E)	0.	0.4724	0.5670	0.7451	0.9192	1.0898	1.2594	1.4296	1.6004	1.6004
SHELL	(5P) 0	(5P) 0	(5P) 0	(5P) 1	(5P) 2	(5P) 3	(5P) 4	(5P) 5	(5P) 6	(5P) 6
(-E)	0.	0.	0.	0.3452	0.4370	0.5337	0.6328	0.7341	0.8368	0.8368
U(X) <th>X</th> <th>CS 55</th> <th>BA 56</th> <th>LA 57</th> <th>CE 58</th> <th>PR 59</th> <th>ND 60</th> <th>PM 61</th> <th>SM 62</th> <th>EU 63</th>	X	CS 55	BA 56	LA 57	CE 58	PR 59	ND 60	PM 61	SM 62	EU 63
	X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000

U(X)	X	CS 55	RA 56	LA 57	CE 58	PR 59	ND 60	PM 61	SM 62	EU 63
00.01	C.98895	C.98897	C.98896	C.98892	0.98889	0.98886	0.98883	0.98880	0.98877	
00.02	C.97777	C.97774	C.97771	C.97764	0.97758	0.97752	0.97747	0.97741	0.97735	
00.03	C.96655	0.96652	0.96648	C.96637	0.96629	0.96621	0.96612	0.96604	0.96596	
00.04	0.95545	0.95542	0.95537	C.95523	0.95513	0.95503	0.95493	0.95483	0.95472	
00.05	C.94454	0.94451	0.94446	C.94429	0.94418	0.94406	0.94394	0.94382	0.94370	
00.06	C.93385	0.93383	0.93378	0.93358	0.93345	0.93332	0.93319	0.93305	0.93292	
00.07	C.92340	0.92338	0.92332	0.92311	0.92297	0.92283	0.92268	0.92253	0.92238	
00.08	C.91317	0.91316	0.91311	C.91288	0.91273	0.91257	0.91242	0.91226	0.91209	
00.09	C.90317	0.90317	C.90313	C.90287	0.90271	0.90255	0.90238	0.90221	0.90204	
00.10	C.89340	0.89340	0.89337	0.89309	0.89293	0.89276	0.89258	0.89240	0.89222	
00.12	C.87449	C.87452	0.87451	0.87420	0.87402	0.87384	0.87365	0.87345	0.87325	
00.14	0.85642	0.85649	0.85649	0.85616	0.85597	0.85578	0.85558	0.85538	0.85517	
00.16	C.83916	0.83927	0.83930	C.83894	0.83876	0.83856	0.83836	0.83815	0.83792	
00.18	C.82268	0.82283	0.82289	0.82250	0.82232	0.82212	0.82191	0.82169	0.82146	
00.20	C.80691	0.80709	0.80718	0.80677	0.80658	0.80638	0.80616	0.80593	0.80569	
00.22	0.79178	0.79200	0.79211	0.79167	0.79147	0.79126	0.79103	0.79078	0.79052	
00.24	C.77721	0.77746	0.77760	0.77712	0.77691	0.77669	0.77644	0.77618	0.77590	
00.26	0.76315	0.76343	0.76358	0.76307	0.76285	0.76261	0.76235	0.76206	0.76176	
00.28	C.74956	0.74986	C.75003	0.74948	0.74925	0.74899	0.74871	0.74841	0.74809	
00.30	0.73638	0.73672	0.73691	0.73632	0.73607	0.73580	0.73550	0.73518	0.73484	
00.34	C.71123	0.71162	0.71184	0.71118	0.71090	0.71060	0.71027	0.70991	0.70953	
00.38	0.68752	0.68797	0.68824	0.68750	0.68720	0.68687	0.68650	0.68611	0.68569	
00.42	0.66513	0.66564	0.66595	C.66514	0.66482	0.66446	0.66407	0.66364	0.66318	
00.46	C.64395	0.64453	0.64489	0.64401	0.64366	0.64328	0.64286	0.64240	0.64191	
00.50	C.62389	0.62454	0.62496	C.62400	0.62364	0.62325	0.62280	0.62232	0.62180	
00.54	C.60488	0.60561	0.60609	0.60507	0.60470	0.60429	0.60383	0.60332	0.60278	
00.58	0.58686	0.58768	0.58823	C.58715	0.58677	0.58635	0.58588	0.58535	0.58479	
00.62	C.56979	0.57070	0.57132	C.57018	0.56980	0.56937	0.56888	0.56834	0.56775	
00.66	C.55360	0.55461	0.55531	C.55410	0.55372	0.55328	0.55277	0.55220	0.55159	
00.70	0.53825	0.53935	0.54012	0.53884	0.53845	0.53800	0.53747	0.53687	0.53622	
00.78	C.50977	0.51105	0.51195	C.51052	0.51010	0.50960	0.50901	0.50835	0.50762	
00.86	C.48387	0.48531	0.48633	0.48474	0.48427	0.48370	0.48304	0.48230	0.48148	
00.94	C.46018	0.46178	0.46292	C.46114	0.46061	0.45998	0.45924	0.45841	0.45749	
01.02	0.43842	0.44018	0.44142	0.43945	0.43885	0.43815	0.43732	0.43639	0.43537	
01.10	C.41840	0.42028	0.42162	C.41945	0.41878	0.41798	0.41706	0.41603	0.41489	
01.18	C.39988	0.40189	0.40331	C.40093	0.40017	0.39927	0.39824	0.39709	0.39584	
01.26	C.38271	0.38482	0.38630	0.38370	0.38283	0.38183	0.38069	0.37942	0.37804	
01.34	C.36670	0.36890	0.37042	0.36759	0.36662	0.36551	0.36425	0.36286	0.36136	
01.42	C.35172	0.35399	0.35554	C.35249	0.35142	0.35019	0.34882	0.34732	0.34572	
01.50	C.33765	0.33999	0.34158	C.33831	0.33713	0.33581	0.33434	0.33275	0.33106	
01.66	C.31196	0.31446	0.31612	0.31246	0.31113	0.30966	0.30804	0.30630	0.30445	
01.82	0.28923	0.29193	C.29372	0.28972	0.28827	0.28666	0.28490	0.28301	0.28100	
01.98	C.26918	0.27209	0.27401	0.26965	0.26805	0.26629	0.26435	0.26228	0.26009	
02.14	0.25141	0.25447	0.25645	0.25171	0.24993	0.24797	0.24584	0.24358	0.24121	
02.30	C.23543	0.23859	C.24057	C.23544	0.23347	0.23132	0.22901	0.22659	0.22407	
02.46	C.22086	0.22409	0.22606	0.22057	0.21842	0.21611	0.21367	0.21112	0.20850	
02.62	C.20749	0.21077	0.21272	C.20693	0.20464	0.20222	0.19968	0.19705	0.19437	
02.78	0.19517	0.19852	0.20046	0.19442	0.19204	0.18954	0.18694	0.18427	0.18157	
02.94	C.18381	0.18724	0.18918	0.18296	0.18051	0.17797	0.17534	0.17267	0.16997	
03.10	C.17335	0.17686	0.17880	0.17245	0.16998	0.16741	0.16479	0.16212	0.15945	
03.42	C.15484	0.15852	0.16047	C.15399	0.15151	0.14897	0.14639	0.14380	0.14122	
03.74	0.13909	0.14292	0.14485	0.13840	0.13596	0.13349	0.13101	0.12853	0.12607	
04.06	C.12562	0.12959	0.13147	0.12515	0.12280	0.12043	0.11807	0.11572	0.11341	
04.38	0.11406	0.11815	0.11999	0.11387	0.11163	0.10938	0.10715	0.10494	0.10277	
04.70	0.10409	0.10834	0.11016	C.10426	0.10213	0.10001	0.09791	0.09583	0.09380	
05.02	0.09551	0.09994	0.10174	C.09605	0.09404	0.09203	0.09004	0.08809	0.08617	
05.34	C.08814	0.09273	C.09450	0.08902	0.08709	0.08518	0.08329	0.08143	0.07962	
05.66	C.08179	0.08650	0.08820	0.08292	0.08107	0.07923	0.07742	0.07565	0.07392	

U(X) X	CS 55	BA 56	LA 57	CE 58	PR 59	ND 60	PM 61	SM 62	EU 63
05.98	0.07627	0.08105	0.08263	0.07796	0.07577	0.07400	0.07225	0.07055	0.06890
06.30	0.07142	0.07622	0.07765	0.07279	0.07105	0.06934	0.06766	0.06602	0.06444
06.94	0.06326	0.06796	0.06902	0.06464	0.06299	0.06138	0.05981	0.05830	0.05685
07.58	0.05656	0.06106	0.06176	0.05786	0.05630	0.05480	0.05334	0.05195	0.05062
08.22	0.05093	0.05518	0.05556	0.05211	0.05066	0.04925	0.04791	0.04663	0.04541
08.86	0.04613	0.05009	0.05022	0.04718	0.04583	0.04452	0.04328	0.04210	0.04098
09.50	0.04198	0.04565	0.04560	0.04291	0.04165	0.04044	0.03930	0.03822	0.03719
10.14	0.03837	0.04176	0.04158	0.03919	0.03801	0.03690	0.03585	0.03486	0.03392
10.78	0.03520	0.03834	0.03810	0.03594	0.03485	0.03383	0.03286	0.03195	0.03110
11.42	0.03239	0.03533	0.03509	0.03311	0.03211	0.03118	0.03029	0.02946	0.02868
12.06	0.02989	0.03272	0.03251	0.03067	0.02976	0.02890	0.02809	0.02734	0.02663
12.70	0.02766	0.03046	0.03031	0.02859	0.02775	0.02697	0.02624	0.02555	0.02491
13.98	0.02391	0.02691	0.02684	0.02534	0.02465	0.02399	0.02338	0.02281	0.02227
15.26	0.02101	0.02438	0.02429	0.02304	0.02245	0.02190	0.02137	0.02088	0.02042
16.54	0.01884	0.02253	0.02232	0.02136	0.02084	0.02034	0.01987	0.01943	0.01902
17.82	0.01818	0.02110	0.02072	0.02002	0.01955	0.01909	0.01866	0.01826	0.01789
19.10	0.01818	0.01989	0.01935	0.01888	0.01845	0.01802	0.01762	0.01724	0.01688
20.38	0.01818	0.01882	0.01814	0.01787	0.01746	0.01705	0.01667	0.01632	0.01598
21.66	0.01818	0.01786	0.01754	0.01724	0.01695	0.01667	0.01639	0.01613	0.01587
22.94	0.01818	0.01786	0.01754	0.01724	0.01695	0.01667	0.01639	0.01613	0.01587
24.22	0.01818	0.01786	0.01754	0.01724	0.01695	0.01667	0.01639	0.01613	0.01587
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(=E)	2530.9	2629.3	2729.5	2830.2	2933.4	3038.5	3145.3	3254.1	3364.6
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(=E)	389.53	407.44	425.55	442.70	460.82	479.28	498.08	517.23	536.72
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(=E)	368.03	385.44	403.04	419.70	437.33	455.29	473.60	492.26	511.25
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(=E)	81.91	87.03	92.07	95.70	100.12	104.59	109.14	113.76	118.45
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(=E)	72.60	77.45	82.23	85.59	89.74	93.95	98.22	102.57	106.98
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(=E)	55.138	59.479	63.743	66.605	70.247	73.944	77.709	81.539	85.438
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(=E)	15.793	17.465	18.970	19.196	20.046	20.894	21.741	22.591	23.444
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(=E)	12.388	13.916	15.378	15.275	16.093	16.804	17.515	18.226	18.939
SHELL (4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(=E)	6.437	7.679	8.751	8.625	9.079	9.528	9.974	10.418	10.862
SHELL (4F) 0	(4F) 0	(4F) 0	(4F) 0	(4F) 2	(4F) 3	(4F) 4	(4F) 5	(4F) 6	(4F) 7
(=E)	0.	0.	0.	0.7446	0.8102	0.8678	0.9191	0.9642	1.0040
SHELL (5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(=E)	2.1187	2.6393	2.9769	2.8258	2.9108	2.9917	3.0717	3.1491	3.2251
SHELL (5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6
(=E)	1.2543	1.6800	1.9372	1.7894	1.8372	1.8814	1.9249	1.9660	2.0057
SHELL (5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0
(=E)	0.	0.	0.4552	0.	0.	0.	0.	0.	0.
SHELL (6S) 1	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2
(=E)	0.2620	0.3280	0.3577	0.3375	0.3417	0.3455	0.3493	0.3530	0.3565
U(X) X	CD 64	TB 65	DY 66	HC 67	ER 68	YM 69	YB 70	LU 71	HF 72
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.98875	0.98871	0.98868	0.98865	0.98862	0.98858	0.98856	0.98853	0.98851
00.02	0.97731	0.97723	0.97717	0.97711	0.97705	0.97699	0.97693	0.97688	0.97685
00.03	0.96591	0.96579	0.96571	0.96562	0.96554	0.96545	0.96536	0.96531	0.96525
00.04	0.95466	0.95451	0.95441	0.95430	0.95419	0.95408	0.95397	0.95390	0.95384
00.05	0.94363	0.94345	0.94333	0.94320	0.94308	0.94294	0.94282	0.94274	0.94266
00.06	0.93284	0.93264	0.93250	0.93236	0.93221	0.93206	0.93192	0.93183	0.93175

U(X)	X	GD 64	TR 65	DY 66	HC 67	ER 68	TM 69	YP 70	LU 71	HF 72
00.07	C.92230	0.92208	0.92192	0.92176	0.92160	0.92143	0.92128	0.92118	0.92109	
00.08	C.91201	0.91176	0.91159	0.91142	0.91124	0.91105	0.91089	0.91079	0.91069	
00.09	C.90195	0.90168	0.90150	0.90132	0.90113	0.90092	0.90074	0.90064	0.90054	
00.10	C.89213	0.89184	0.89164	0.89145	0.89125	0.89103	0.89084	0.89073	0.89062	
00.12	C.87317	0.87284	0.87262	0.87241	0.87218	0.87194	0.87173	0.87162	0.87151	
00.14	0.85510	0.85472	0.85450	0.85427	0.85403	0.85376	0.85354	0.85343	0.85332	
00.16	C.83787	0.83746	0.83722	0.83698	0.83672	0.83644	0.83620	0.83609	0.83598	
00.18	C.82141	0.82097	0.82072	0.82046	0.82018	0.81987	0.81962	0.81950	0.81940	
00.20	C.80565	0.80517	0.80489	0.80461	0.80431	0.80398	0.80370	0.80359	0.80347	
00.22	0.79048	0.78996	0.78967	0.78937	0.78904	0.78868	0.78838	0.78825	0.78813	
00.24	C.77586	0.77530	0.77498	0.77465	0.77430	0.77391	0.77358	0.77345	0.77332	
00.26	C.76173	0.76112	0.76077	0.76042	0.76004	0.75962	0.75927	0.75913	0.75899	
00.28	0.74805	0.74739	0.74703	0.74665	0.74624	0.74579	0.74541	0.74526	0.74512	
00.30	C.73480	0.73410	0.73370	0.73330	0.73287	0.73239	0.73198	0.73182	0.73167	
00.34	C.70950	0.70870	0.70826	C.70781	0.70732	0.70678	0.70632	0.70615	0.70599	
00.38	C.68567	0.68477	0.68429	0.68379	0.68325	0.68265	0.68214	0.68196	0.68178	
00.42	C.66317	0.66219	0.66166	C.66111	0.66052	0.65987	0.65931	0.65912	0.65894	
00.46	C.64192	0.64085	0.64027	0.63969	0.63905	0.63834	0.63774	0.63755	0.63737	
00.50	0.62183	0.62067	0.62006	0.61944	0.61876	0.61800	0.61736	0.61717	0.61699	
00.54	C.60283	0.60159	0.60095	0.60029	0.59957	0.59877	0.59809	0.59790	0.59772	
00.58	C.58487	0.58354	0.58287	0.58217	0.58141	0.58056	0.57984	0.57965	0.57947	
00.62	C.56786	0.56644	0.56573	0.56500	0.56419	0.56328	0.56252	0.56232	0.56214	
00.66	C.55172	0.55021	0.54945	0.54868	0.54782	0.54686	0.54604	0.54584	0.54565	
00.70	0.53637	0.53476	0.53396	0.53314	0.53223	0.53120	0.53033	0.53012	0.52993	
00.78	C.50779	0.50598	0.50507	0.50414	0.50311	0.50196	0.50097	0.50073	0.50051	
00.86	0.48168	0.47964	0.47863	0.47758	0.47643	0.47514	0.47403	0.47376	0.47351	
00.94	C.45770	0.45543	0.45430	0.45314	0.45185	0.45043	0.44919	0.44889	0.44861	
01.02	C.43559	0.43309	0.43183	0.43054	0.42912	0.42756	0.42619	0.42585	0.42554	
01.10	C.41510	0.41236	0.41098	0.40956	0.40800	0.40629	0.40479	0.40442	0.40407	
01.18	C.39603	0.39305	0.39154	0.38999	0.38830	0.38645	0.38483	0.38442	0.38405	
01.26	C.37821	0.37500	0.37336	0.37169	0.36988	0.36790	0.36616	0.36574	0.36536	
01.34	0.36152	0.35809	0.35634	0.35455	0.35263	0.35055	0.34871	0.34828	0.34790	
01.42	C.34588	0.34224	0.34039	0.33851	0.33650	0.33432	0.33239	0.33197	0.33160	
01.50	C.33122	0.32740	0.32547	0.32350	0.32140	0.31913	0.31713	0.31672	0.31636	
01.66	C.30466	0.30048	0.29839	0.29626	0.29399	0.29156	0.28939	0.28899	0.28866	
01.82	C.28125	0.27670	0.27443	0.27213	0.26969	0.26708	0.26475	0.26437	0.26405	
01.98	C.26033	0.25542	0.25298	0.25051	0.24791	0.24515	0.24269	0.24235	0.24209	
02.14	0.24145	0.23621	0.23362	0.23103	0.22831	0.22546	0.22291	0.22265	0.22247	
02.30	C.22432	0.21883	0.21614	0.21347	0.21068	0.20778	0.20521	0.20506	0.20501	
02.46	C.20880	0.20310	0.20037	0.19766	0.19487	0.19197	0.18940	0.18940	0.18947	
02.62	0.19474	0.18891	0.18617	0.18347	0.18069	0.17783	0.17530	0.17545	0.17567	
02.78	C.18203	0.17611	0.17339	0.17072	0.16799	0.16519	0.16272	0.16302	0.16337	
02.94	C.17052	0.16456	0.16189	0.15927	0.15660	0.15398	0.15148	0.15192	0.15239	
03.10	C.16009	0.15413	0.15151	0.14896	0.14637	0.14373	0.14140	0.14197	0.14255	
03.42	0.14202	0.13614	0.13366	0.13126	0.12883	0.12638	0.12421	0.12500	0.12573	
03.74	C.12699	0.12128	0.11896	0.11672	0.11446	0.11219	0.11018	0.11114	0.11198	
04.06	0.11442	0.10892	0.10676	0.10468	0.10258	0.10049	0.09864	0.09972	0.10063	
04.38	C.10386	0.09858	0.09657	0.09464	0.09270	0.09077	0.08905	0.09022	0.09117	
04.70	C.09494	0.08988	0.08800	0.08621	0.08440	0.08261	0.08101	0.08223	0.08317	
05.02	C.08733	0.08249	0.08073	0.07904	0.07736	0.07569	0.07419	0.07542	0.07632	
05.34	C.08076	0.07614	0.07447	0.07289	0.07130	0.06974	0.06832	0.06954	0.07038	
05.66	C.07500	0.07061	0.06903	0.06753	0.06603	0.06456	0.06323	0.06441	0.06517	
05.98	C.06991	0.06575	0.06425	0.06283	0.06141	0.06003	0.05877	0.05989	0.06056	
06.30	C.06537	0.06143	0.06001	0.05866	0.05732	0.05601	0.05482	0.05587	0.05645	
06.94	0.05758	0.05411	0.05282	0.05160	0.05040	0.04923	0.04816	0.04905	0.04946	
07.58	C.05116	0.04812	0.04695	0.04585	0.04476	0.04372	0.04275	0.04349	0.04375	
08.22	0.04578	0.04313	0.04207	0.04107	0.04009	0.03915	0.03827	0.03888	0.03903	
08.86	C.04123	0.03891	0.03794	C.03704	0.03614	0.03529	0.03450	0.03501	0.03508	

U(X) X	GD 64	TR 65	DY 66	HC 67	ER 68	TM 69	YB 70	LU 71	HF 72
09.50	0.03736	0.03529	0.03442	0.03359	0.03278	0.03201	0.03129	0.03174	0.03178
10.14	0.03405	0.03219	0.03139	0.03064	0.02990	0.02921	0.02855	0.02899	0.02901
10.78	0.03123	0.02952	0.02880	0.02812	0.02745	0.02682	0.02622	0.02667	0.02670
11.42	0.02885	0.02725	0.02659	0.02597	0.02537	0.02480	0.02426	0.02474	0.02476
12.06	0.02684	0.02533	0.02473	0.02418	0.02363	0.02311	0.02262	0.02312	0.02313
12.70	0.02515	0.02373	0.02318	0.02268	0.02218	0.02171	0.02127	0.02177	0.02175
13.98	0.02251	0.02129	0.02083	0.02040	0.01998	0.01959	0.01921	0.01964	0.01952
15.26	0.02054	0.01956	0.01916	0.01879	0.01842	0.01808	0.01774	0.01802	0.01778
16.54	0.01898	0.01825	0.01785	0.01755	0.01722	0.01690	0.01659	0.01669	0.01634
17.82	0.01767	0.01716	0.01683	0.01652	0.01620	0.01591	0.01562	0.01555	0.01510
19.10	0.01652	0.01621	0.01590	0.01560	0.01531	0.01504	0.01476	0.01453	0.01402
20.38	0.01562	0.01538	0.01515	0.01493	0.01471	0.01449	0.01429	0.01408	0.01389
21.66	0.01562	0.01538	0.01515	0.01493	0.01471	0.01449	0.01429	0.01408	0.01389
22.94	0.01562	0.01538	0.01515	0.01493	0.01471	0.01449	0.01429	0.01408	0.01389
24.22	0.01562	0.01538	0.01515	0.01493	0.01471	0.01449	0.01429	0.01408	0.01389
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(-E)	3477.7	3591.3	3707.4	3825.4	3945.2	4066.9	4190.3	4316.4	444.3
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(-E)	557.23	576.74	597.27	618.14	639.38	661.00	682.89	705.89	729.27
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(-E)	531.26	550.29	570.32	590.70	611.44	632.57	653.96	676.45	699.33
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(-E)	123.95	128.04	132.96	137.94	143.01	148.19	153.38	159.46	165.68
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(-E)	112.21	116.03	120.66	125.36	130.16	135.06	139.96	145.75	151.68
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(-E)	90.14	93.44	97.56	101.73	106.00	110.37	114.74	119.99	125.37
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(-E)	24.956	25.165	26.034	26.907	27.797	28.702	29.593	31.211	32.878
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(-E)	20.302	20.377	21.102	21.829	22.572	23.328	24.069	25.530	27.037
SHELL (4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(-E)	11.933	11.751	12.196	12.642	13.099	13.565	14.013	15.164	16.355
SHELL (4F) 7	(4F) 9	(4F) 10	(4F) 11	(4F) 11	(4F) 12	(4F) 13	(4F) 14	(4F) 14	(4F) 14
(-E)	1.5912	1.0702	1.0968	1.1170	1.1418	1.1677	1.1748	1.8092	2.4819
SHELL (5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(-E)	3.5683	3.3743	3.4480	3.5194	3.5937	3.6651	3.7389	4.1225	4.4903
SHELL (5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6
(-E)	2.2693	2.0819	2.1189	2.1538	2.1908	2.2248	2.2612	2.5588	2.8401
SHELL (5D) 1	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 0	(5D) 1	(5D) 2
(-E)	0.4363	0.	0.	0.	0.	0.	0.	0.3905	0.4902
SHELL (6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2
(-E)	0.3878	0.3633	0.3666	0.3697	0.3731	0.3759	0.3794	0.4160	0.4437
U(X) X	TA 73	W 74	RE 75	OS 76	IR 77	PT 78	AU 79	FG 80	TL 81
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.98845	0.98847	0.98845	0.98843	0.98841	0.98839	0.98837	0.98835	0.98834
00.02	0.97681	0.97677	0.97673	0.97669	0.97665	0.97661	0.97657	0.97654	0.97652
00.03	0.96520	0.96514	0.96509	0.96503	0.96498	0.96491	0.96486	0.96482	0.96479
00.04	0.95377	0.95370	0.95363	0.95357	0.95350	0.95342	0.95336	0.95331	0.95327
00.05	0.94258	0.94251	0.94243	0.94236	0.94228	0.94219	0.94212	0.94206	0.94202
00.06	0.93166	0.93158	0.93149	0.93141	0.93133	0.93122	0.93114	0.93109	0.93104
00.07	0.92100	0.92091	0.92082	0.92073	0.92064	0.92052	0.92044	0.92038	0.92033
00.08	0.91059	0.91049	0.91040	0.91030	0.91021	0.91008	0.90999	0.90993	0.90989
00.09	0.90043	0.90033	0.90023	0.90013	0.90003	0.89990	0.89980	0.89974	0.89970
00.10	0.89052	0.89041	0.89031	0.89021	0.89011	0.88996	0.88986	0.88981	0.88977
00.12	0.87140	0.87130	0.87119	0.87109	0.87098	0.87082	0.87072	0.87067	0.87064
00.14	0.85321	0.85310	0.85300	0.85289	0.85279	0.85262	0.85252	0.85247	0.85245

U(X)	X	TA 73	W 74	RE 75	CS 76	IR 77	PT 78	AU 79	FC 80	IL 81
00.16	C.83587	0.83576	0.83566	C.83555	0.83544	0.83527	0.83516	0.83512	0.83511	
00.18	C.81928	0.81917	0.81907	0.81895	0.81884	0.81865	0.81854	0.81850	0.81850	
00.20	C.80336	0.80324	0.80312	0.80301	0.80289	0.80268	0.80256	0.80253	0.80253	
00.22	0.78801	0.78788	0.78776	C.78764	0.78751	0.78728	0.78716	0.78712	0.78712	
00.24	C.77319	0.77305	0.77292	0.77279	0.77265	0.77241	0.77227	0.77223	0.77224	
00.26	C.75885	0.75871	0.75857	C.75843	0.75828	0.75802	0.75787	0.75784	0.75785	
00.28	0.74497	0.74482	0.74467	0.74452	0.74437	0.74409	0.74393	0.74390	0.74391	
00.30	C.73151	0.73136	0.73120	0.73105	0.73089	0.73059	0.73043	0.73039	0.73042	
00.34	0.70582	0.70565	0.70548	C.70531	0.70514	0.70481	0.70464	0.70461	0.70464	
00.38	0.68160	0.68142	0.68125	C.68107	0.68089	0.68054	0.68035	0.68033	0.68039	
00.42	C.65875	0.65857	0.65839	0.65821	0.65802	0.65765	0.65746	0.65746	0.65753	
00.46	C.63718	0.63700	0.63682	0.63663	0.63645	0.63606	0.63587	0.63589	0.63599	
00.50	C.61680	0.61662	0.61645	0.61627	0.61609	0.61568	0.61549	0.61553	0.61566	
00.54	C.59754	0.59736	0.59718	0.59701	0.59683	0.59641	0.59622	0.59627	0.59643	
00.58	C.57929	0.57911	0.57893	0.57876	0.57858	0.57814	0.57795	0.57801	0.57819	
00.62	0.56196	0.56178	0.56160	0.56142	0.56123	0.56077	0.56057	0.56065	0.56085	
00.66	0.54546	0.54527	0.54509	C.54490	0.54471	0.54422	0.54401	0.54410	0.54432	
00.70	C.52972	0.52952	0.52933	0.52913	0.52893	0.52842	0.52820	0.52830	0.52853	
00.78	0.50029	0.50007	0.49985	C.49963	0.49942	0.49885	0.49861	0.49872	0.49898	
00.86	C.47326	0.47302	0.47278	0.47254	0.47229	0.47167	0.47141	0.47153	0.47182	
00.94	C.44833	0.44806	0.44779	0.44752	0.44726	0.44657	0.44628	0.44642	0.44674	
01.02	0.42522	0.42492	0.42463	C.42434	0.42404	0.42330	0.42299	0.42314	0.42349	
01.10	C.40373	0.40340	0.40308	0.40277	0.40246	0.40167	0.40135	0.40152	0.40191	
01.18	C.38368	0.38334	0.38301	0.38269	0.38238	0.38155	0.38122	0.38144	0.38188	
01.26	C.36498	0.36464	0.36431	C.36399	0.36369	0.36283	0.36251	0.36278	0.36328	
01.34	C.34753	0.34719	0.34688	0.34658	0.34629	0.34541	0.34510	0.34542	0.34599	
01.42	0.33124	0.33092	0.33062	0.33034	0.33006	0.32917	0.32887	0.32923	0.32986	
01.50	C.31602	0.31571	0.31543	C.31516	0.31489	0.31397	0.31368	0.31409	0.31478	
01.66	C.28833	0.28805	0.28779	0.28754	0.28730	0.28633	0.28606	0.28656	0.28738	
01.82	C.26376	0.26350	0.26328	0.26307	0.26287	0.26188	0.26165	0.26227	0.26323	
01.98	C.24184	0.24166	0.24150	0.24136	0.24123	0.24024	0.24008	0.24083	0.24195	
02.14	C.22232	0.22223	0.22217	0.22212	0.22208	0.22112	0.22103	0.22193	0.22321	
02.30	C.20498	0.20500	0.20505	C.20510	0.20516	0.20421	0.20419	0.20521	0.20664	
02.46	0.18957	0.18972	0.18988	0.19003	0.19017	0.18921	0.18925	0.19038	0.19193	
02.62	C.17589	0.17615	0.17640	0.17663	0.17684	0.17586	0.17592	0.17713	0.17878	
02.78	C.16371	0.16406	0.16440	0.16468	0.16492	0.16390	0.16396	0.16524	0.16697	
02.94	C.15283	0.15326	0.15364	0.15397	0.15423	0.15313	0.15318	0.15451	0.15631	
03.10	C.14307	0.14355	0.14398	0.14432	0.14458	0.14340	0.14343	0.14480	0.14666	
03.42	0.12636	0.12692	0.12737	0.12772	0.12795	0.12658	0.12655	0.12800	0.12999	
03.74	C.11268	0.11326	0.11371	C.11403	0.11422	0.11264	0.11253	0.11404	0.11613	
04.06	C.10135	0.10193	0.10235	C.10261	0.10273	0.10093	0.10072	0.10225	0.10439	
04.38	C.09188	0.09242	0.09278	0.09296	0.09297	0.09093	0.09059	0.09210	0.09427	
04.70	C.08384	0.08431	0.08458	C.08465	0.08454	0.08226	0.08178	0.08326	0.08544	
05.02	0.07693	0.07730	0.07746	C.07741	0.07717	0.07466	0.07406	0.07551	0.07770	
05.34	C.07090	0.07117	C.07121	0.07104	0.07068	0.06798	0.06727	0.06869	0.07090	
05.66	0.06559	0.06575	0.06568	C.06540	0.06494	0.06208	0.06128	0.06269	0.06491	
05.98	C.06088	0.06094	0.06076	C.06038	0.05983	0.05686	0.05600	0.05739	0.05963	
06.30	C.05668	0.05664	0.05637	0.05591	0.05529	0.05224	0.05134	0.05272	0.05498	
06.94	C.04952	0.04932	0.04892	0.04834	0.04763	0.04451	0.04359	0.04494	0.04720	
07.58	C.04368	0.04338	0.04288	0.04224	0.04148	0.03841	0.03749	0.03880	0.04105	
08.22	C.03886	0.03849	0.03795	0.03728	0.03651	0.03353	0.03265	0.03391	0.03613	
08.86	C.03487	0.03446	0.03389	0.03322	0.03246	0.02960	0.02876	0.02997	0.03215	
09.50	C.03154	0.03111	0.03054	C.02987	0.02914	0.02640	0.02561	0.02677	0.02891	
10.14	0.02876	0.02833	C.02776	C.02710	0.02639	0.02376	0.02301	0.02415	0.02624	
10.78	C.02644	0.02600	0.02543	0.02479	0.02409	0.02156	0.02086	0.02197	0.02403	
11.42	C.02449	0.02404	C.02347	0.02284	0.02216	0.01971	0.01904	0.02015	0.02217	
12.06	C.02284	0.02238	0.02180	0.02118	0.02053	0.01814	0.01750	0.01860	0.02059	
12.70	C.02143	0.02095	0.02037	C.01975	0.01912	0.01680	0.01619	0.01729	0.01924	

U(X)	X	TA 73	W 74	RE 75	GS 76	IR 77	PT 78	AU 79	HC 80	TL 81
13.98	C.01913	0.01862	0.01803	0.01743	0.01683	0.01462	0.01407	0.01517	0.01701	
15.26	0.01732	0.01677	0.01618	0.01560	0.01504	0.01296	0.01266	0.01353	0.01526	
16.54	0.01582	0.01525	0.01467	0.01412	0.01359	0.01282	0.01266	0.01250	0.01382	
17.82	0.01454	0.01397	0.01340	0.01316	0.01299	0.01282	0.01266	0.01250	0.01262	
19.10	C.01370	0.01351	0.01333	0.01316	0.01299	0.01282	0.01266	0.01250	0.01235	
20.38	C.01370	0.01351	0.01333	0.01316	0.01299	0.01282	0.01266	0.01250	0.01235	
21.66	0.01370	0.01351	0.01333	0.01316	0.01299	0.01282	0.01266	0.01250	0.01235	
22.94	C.01370	0.01351	0.01333	0.01316	0.01299	0.01282	0.01266	0.01250	0.01235	
24.22	0.01370	0.01351	0.01333	0.01316	0.01299	0.01282	0.01266	0.01250	0.01235	
SHELL	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	
(=E)	4574.0	4705.8	4839.4	4974.9	5112.3	5251.3	5392.1	5535.7	5681.5	
SHELL	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	
(=E)	753.08	777.29	801.90	826.92	852.34	877.83	903.98	930.98	958.55	
SHELL	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	
(=E)	722.62	746.32	770.42	794.92	819.83	844.80	870.43	896.92	923.96	
SHELL	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	
(=E)	172.04	178.55	185.20	191.99	198.92	205.65	212.81	220.49	228.47	
SHELL	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	
(=E)	157.75	163.97	170.33	176.82	183.45	189.88	196.75	204.12	211.80	
SHELL	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	
(=E)	130.89	136.56	142.36	148.29	154.35	160.22	166.52	173.33	180.43	
SHELL	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	
(=E)	34.597	36.367	38.185	40.048	41.956	43.580	45.557	47.934	50.513	
SHELL	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	
(=E)	28.594	30.199	31.851	33.547	35.287	36.740	38.546	40.746	43.155	
SHELL	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	
(=E)	17.593	18.875	20.201	21.568	22.976	24.095	25.565	27.430	29.495	
SHELL	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	
(=E)	3.199	3.961	4.765	5.610	6.497	7.095	8.044	9.386	10.927	
SHELL	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	
(=E)	4.8525	5.2126	5.5715	5.9297	6.2892	6.3498	6.6945	7.3714	8.1999	
SHELL	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	
(=E)	3.1151	3.3875	3.6583	3.9281	4.1986	4.1816	4.4370	5.0123	5.7368	
SHELL	(5D) 3	(5D) 4	(5D) 5	(5D) 6	(5D) 7	(5D) 10	(5D) 10	(5D) 10	(5D) 10	
(=E)	0.5875	0.6841	0.7806	0.8771	0.9745	0.873	0.9200	1.2703	1.7644	
SHELL	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 1	(6S) 1	(6S) 2	(6S) 2	
(=E)	0.4664	0.4858	0.5027	0.5177	0.5311	0.4693	0.4775	0.5653	0.7302	
SHELL	(6P) 0	(6P) 0	(6P) 0	(6P) 0	(6P) 0	(6P) 0	(6P) 0	(6P) 0	(6P) 1	
(=E)	0.	0.	0.	0.	0.	0.	0.	0.	0.3393	

U(X)	X	PB 82	BI 83	PO 84	AT 85	RN 86	FR 87	PA 88	AC 89	TH 90
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
01.01	0.98832	0.98831	0.98830	0.98829	0.98827	0.98827	0.98826	0.98825	0.98824	
00.02	C.97645	0.97647	0.97644	C.97642	0.97640	0.97639	0.97637	0.97636	0.97634	
00.03	0.96476	0.96473	0.96469	C.96466	0.96463	0.96462	0.96460	0.96458	0.96456	
00.04	0.95324	0.95320	0.95316	0.95313	0.95310	0.95308	0.95306	0.95304	0.95302	
00.05	0.94198	0.94194	0.94190	C.94187	0.94183	0.94181	0.94180	0.94178	0.94176	
00.06	0.93100	0.93096	0.93092	C.93088	0.93084	0.93083	0.93082	0.93080	0.93078	
00.07	C.92029	0.92025	0.92021	C.92017	0.92013	0.92013	0.92012	0.92010	0.92009	
00.08	C.90985	0.90981	0.90977	0.90973	0.90969	0.90969	0.90969	0.90968	0.90966	
00.09	C.89966	0.89962	0.89959	0.89955	0.89952	0.89952	0.89953	0.89952	0.89951	
00.10	0.88973	0.88969	0.88966	0.88963	0.88960	0.88961	0.88962	0.88962	0.88962	
00.12	0.87061	0.87059	0.87056	C.87054	0.87052	0.87055	0.87058	0.87059	0.87060	
00.14	0.85244	0.85242	0.85241	0.85239	0.85238	0.85243	0.85248	0.85251	0.85253	
00.16	0.83510	0.83510	0.83509	C.83508	0.83508	0.83515	0.83522	0.83525	0.83529	
00.18	0.81850	0.81850	0.81850	0.81850	0.81850	0.81858	0.81866	0.81871	0.81875	
00.20	0.80253	0.80253	0.80254	0.80254	0.80255	0.80264	0.80273	0.80279	0.80284	
00.22	0.78713	0.78713	0.78714	0.78715	0.78716	0.78726	0.78737	0.78744	0.78749	

U(X)	X	PR 82	BI 83	PO 84	AT 85	RN 86	FR 87	RA 88	AC 89	TH 90
00.24	0.77225	0.77226	0.77227	0.77228	0.77230	0.77241	0.77254	0.77261	0.77267	
00.26	0.75786	0.75787	0.75789	0.75791	0.75793	0.75806	0.75819	0.75827	0.75835	
00.28	0.74393	0.74395	0.74397	0.74399	0.74402	0.74416	0.74431	0.74440	0.74449	
00.30	0.73044	0.73046	0.73049	0.73052	0.73055	0.73071	0.73087	0.73097	0.73107	
00.34	0.70468	0.70472	0.70476	0.70480	0.70485	0.70504	0.70524	0.70536	0.70548	
00.38	0.68044	0.68049	0.68055	0.68062	0.68068	0.68091	0.68115	0.68130	0.68145	
00.42	0.65761	0.65769	0.65777	0.65786	0.65795	0.65822	0.65849	0.65869	0.65887	
00.46	0.63609	0.63620	0.63631	0.63642	0.63654	0.63685	0.63717	0.63740	0.63761	
00.50	0.61578	0.61592	0.61605	0.61619	0.61633	0.61669	0.61705	0.61731	0.61756	
00.54	0.59658	0.59674	0.59689	0.59706	0.59722	0.59762	0.59802	0.59831	0.59858	
00.58	0.57836	0.57854	0.57872	0.57890	0.57908	0.57952	0.57995	0.58027	0.58057	
00.62	0.56103	0.56123	0.56143	0.56163	0.56183	0.56230	0.56277	0.56311	0.56344	
00.66	0.54452	0.54473	0.54495	0.54516	0.54538	0.54588	0.54638	0.54675	0.54710	
00.70	0.52875	0.52898	0.52921	0.52944	0.52967	0.53020	0.53074	0.53113	0.53151	
00.78	0.49923	0.49949	0.49974	0.50001	0.50027	0.50086	0.50147	0.50191	0.50233	
00.86	0.47209	0.47238	0.47266	0.47295	0.47324	0.47390	0.47457	0.47505	0.47552	
00.94	0.44703	0.44735	0.44766	0.44798	0.44830	0.44903	0.44976	0.45030	0.45082	
01.02	0.42382	0.42417	0.42452	0.42487	0.42524	0.42604	0.42685	0.42745	0.42803	
01.10	0.40229	0.40268	0.40308	0.40348	0.40390	0.40479	0.40568	0.40636	0.40701	
01.18	0.38231	0.38276	0.38322	0.38368	0.38416	0.38514	0.38613	0.38688	0.38761	
01.26	0.36377	0.36428	0.36480	0.36533	0.36586	0.36694	0.36802	0.36885	0.36965	
01.34	0.34654	0.34711	0.34769	0.34828	0.34887	0.35003	0.35120	0.35210	0.35297	
01.42	0.33047	0.33110	0.33174	0.33238	0.33303	0.33428	0.33554	0.33651	0.33744	
01.50	0.31545	0.31614	0.31683	0.31752	0.31823	0.31957	0.32092	0.32196	0.32296	
01.66	0.28817	0.28898	0.28979	0.29061	0.29144	0.29297	0.29450	0.29570	0.29685	
01.82	0.26416	0.26511	0.26606	0.26702	0.26798	0.26971	0.27144	0.27279	0.27408	
01.98	0.24304	0.24414	0.24524	0.24633	0.24742	0.24934	0.25125	0.25273	0.25415	
02.14	0.22445	0.22569	0.22691	0.22813	0.22933	0.23141	0.23347	0.23507	0.23659	
02.30	0.20802	0.20937	0.21070	0.21201	0.21330	0.21552	0.21771	0.21940	0.22099	
02.46	0.19341	0.19486	0.19627	0.19765	0.19899	0.20133	0.20364	0.20540	0.20706	
02.62	0.18035	0.18186	0.18334	0.18478	0.18617	0.18862	0.19103	0.19286	0.19458	
02.78	0.16860	0.17018	0.17171	0.17319	0.17463	0.17719	0.17971	0.18161	0.18340	
02.94	0.15800	0.15964	0.16122	0.16275	0.16424	0.16691	0.16953	0.17150	0.17333	
03.10	0.14842	0.15011	0.15174	0.15333	0.15485	0.15762	0.16034	0.16235	0.16422	
03.42	0.13186	0.13364	0.13536	0.13700	0.13857	0.14149	0.14433	0.14638	0.14827	
03.74	0.11807	0.11990	0.12164	0.12328	0.12482	0.12783	0.13074	0.13278	0.13462	
04.06	0.10635	0.10818	0.10990	0.11149	0.11298	0.11604	0.11898	0.12097	0.12275	
04.38	0.09622	0.09803	0.09969	0.10123	0.10264	0.10574	0.10870	0.11065	0.11235	
04.70	0.08738	0.08915	0.09077	0.09224	0.09356	0.09670	0.09968	0.10157	0.10320	
05.02	0.07967	0.08136	0.08293	0.08432	0.08556	0.08873	0.09172	0.09355	0.09510	
05.34	0.07281	0.07451	0.07602	0.07734	0.07848	0.08168	0.08469	0.08645	0.08792	
05.66	0.06681	0.06847	0.06991	0.07116	0.07220	0.07542	0.07845	0.08015	0.08155	
05.98	0.06152	0.06313	0.06451	0.06566	0.06661	0.06987	0.07293	0.07458	0.07591	
06.30	0.05684	0.05839	0.05970	0.06077	0.06163	0.06493	0.06803	0.06964	0.07091	
06.94	0.04899	0.05043	0.05159	0.05252	0.05324	0.05666	0.05985	0.06138	0.06255	
07.58	0.04275	0.04407	0.04512	0.04594	0.04657	0.05013	0.05338	0.05480	0.05582	
08.22	0.03774	0.03896	0.03992	0.04067	0.04123	0.04488	0.04814	0.04940	0.05024	
08.86	0.03368	0.03484	0.03573	0.03641	0.03687	0.04057	0.04377	0.04484	0.04548	
09.50	0.03038	0.03148	0.03231	0.03289	0.03324	0.03694	0.04003	0.04090	0.04135	
10.14	0.02766	0.02870	0.02945	0.02993	0.03016	0.03382	0.03677	0.03746	0.03774	
10.78	0.02540	0.02638	0.02703	0.02740	0.02750	0.03111	0.03390	0.03442	0.03456	
11.42	0.02350	0.02440	0.02495	0.02520	0.02518	0.02872	0.03135	0.03173	0.03176	
12.06	0.02186	0.02268	0.02312	0.02326	0.02315	0.02660	0.02906	0.02933	0.02928	
12.70	0.02044	0.02117	0.02151	0.02155	0.02135	0.02471	0.02701	0.02719	0.02708	
13.58	0.01808	0.01862	0.01878	0.01865	0.01833	0.02147	0.02350	0.02360	0.02344	
15.26	0.01618	0.01655	0.01655	0.01630	0.01588	0.01881	0.02068	0.02078	0.02061	
16.54	0.01459	0.01481	0.01469	0.01435	0.01388	0.01659	0.01847	0.01860	0.01842	
17.82	0.01325	0.01334	0.01311	0.01271	0.01220	0.01477	0.01677	0.01691	0.01672	

U(X) X	PA 82	BI 83	PO 84	AT 85	RN 86	FR 87	RA 88	AC 89	TH 90
19.10	0.01220	0.01208	0.01190	0.01176	0.01163	0.01329	0.01548	0.01559	0.01535
20.38	0.01220	0.01205	0.01190	0.01176	0.01163	0.01214	0.01449	0.01451	0.01422
21.66	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01368	0.01361	0.01326
22.94	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01300	0.01283	0.01242
24.22	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01239	0.01213	0.01167
25.50	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01184	0.01149	0.01111
28.06	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01136	0.01124	0.01111
30.62	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01136	0.01124	0.01111
33.18	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01136	0.01124	0.01111
35.74	0.01220	0.01205	0.01190	0.01176	0.01163	0.01149	0.01136	0.01124	0.01111
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(=E) 5828.9	5978.1	6129.5	6282.6	6437.8	6595.2	6754.1	6915.0	7077.8	
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(=E) 986.5	1014.9	1043.7	1073.0	1102.7	1133.1	1164.0	1195.2	1226.8	
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(=E) 951.4	979.2	1007.5	1036.3	1065.4	1095.4	1125.8	1156.4	1187.5	
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(=E) 236.59	244.87	253.31	261.91	270.67	279.97	289.43	298.89	308.49	
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(=E) 219.61	227.59	235.72	244.02	252.48	261.46	270.62	279.77	289.06	
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(=E) 187.67	195.07	202.63	210.35	218.22	226.62	235.20	243.77	252.48	
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(=E) 53.147	55.847	58.611	61.443	64.342	67.675	71.087	74.394	77.750	
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(=E) 45.614	48.137	50.724	53.377	56.097	59.249	62.481	65.607	68.780	
SHELL (4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(=E) 31.612	33.790	36.032	38.338	40.708	43.510	46.392	49.165	51.985	
SHELL (4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14
(=E) 12.521	14.175	15.893	17.674	19.520	21.797	24.154	26.402	28.697	
SHELL (5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(=E) 9.030	9.874	10.736	11.617	12.517	13.802	15.118	16.281	17.447	
SHELL (5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6
(=E) 6.461	7.198	7.952	8.724	9.515	10.689	11.895	12.946	14.000	
SHELL (5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10
(=E) 2.2588	2.7670	3.2927	3.8377	4.4020	5.3476	6.3248	7.1470	7.9729	
SHELL (6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2
(=E) 0.8889	1.0423	1.1934	1.3435	1.4930	1.9516	2.4019	2.6951	2.9759	
SHELL (6P) 2	(6P) 3	(6P) 4	(6P) 5	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6
(=E) 0.4246	0.5133	0.6035	0.6948	0.7867	1.1573	1.5258	1.7506	1.9652	
SHELL (6D) 0	(6D) 0	(6D) 0	(6D) 0	(6D) 0	(6D) 0	(6D) 0	(6D) 0	(6D) 1	(6D) 2
(=E) 0.	0.	0.	0.	0.	0.	0.	0.4294	0.5158	
SHELL (7S) 0	(7S) 0	(7S) 0	(7S) 0	(7S) 0	(7S) 0	(7S) 1	(7S) 2	(7S) 2	(7S) 2
(=E) 0.	0.	0.	0.	0.	0.	0.2506	0.3119	0.3408	0.3642
U(X) X	PA 91	U 92	NP 93	PU 94	AM 95	CM 96	BK 97	CF 98	E 99
X	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)	U(X)
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.98822	0.98821	0.98819	0.98817	0.98816	0.98815	0.98813	0.98812	0.98810
00.02	0.97630	0.97628	0.97625	0.97621	0.97619	0.97617	0.97614	0.97611	0.97608
00.03	0.96451	0.96447	0.96444	0.96439	0.96435	0.96433	0.96429	0.96425	0.96421
00.04	0.95296	0.95292	0.95287	0.95281	0.95276	0.95274	0.95269	0.95264	0.95260
00.05	0.94165	0.94164	0.94159	0.94152	0.94147	0.94144	0.94139	0.94133	0.94128
00.06	0.93070	0.93065	0.93060	0.93052	0.93046	0.93043	0.93037	0.93032	0.93026
00.07	0.92000	0.91995	0.91989	0.91980	0.91974	0.91971	0.91965	0.91959	0.91952
00.08	0.90957	0.90951	0.90946	0.90936	0.90930	0.90927	0.90921	0.90914	0.90907
00.09	0.89941	0.89935	0.89929	0.89919	0.89913	0.89910	0.89904	0.89897	0.89890
00.10	0.88951	0.88946	0.88940	0.88929	0.88923	0.88921	0.88914	0.88907	0.88900
00.12	0.87045	0.87044	0.87038	0.87026	0.87020	0.87019	0.87012	0.87005	0.86997

U(X)	X	PA 91	U 92	NP 93	PU 94	AM 95	CM 96	BK 97	CF 98	E 99
00.14	C.85242	0.85236	0.85231	0.85218	0.85212	0.85211	0.85204	0.85197	0.85189	
00.16	C.83516	0.83511	0.83505	0.83491	0.83485	0.83485	0.83477	0.83469	0.83461	
00.18	C.81862	0.81856	0.81850	0.81835	0.81827	0.81828	0.81820	0.81811	0.81802	
00.20	C.80269	0.80263	0.80257	0.80240	0.80232	0.80233	0.80224	0.80215	0.80205	
00.22	C.78734	0.78727	0.78720	0.78702	0.78693	0.78695	0.78685	0.78675	0.78664	
00.24	C.77250	0.77244	0.77236	0.77217	0.77208	0.77209	0.77199	0.77188	0.77177	
00.26	C.75816	0.75810	0.75802	0.75781	0.75771	0.75773	0.75763	0.75751	0.75739	
00.28	C.74429	0.74422	0.74414	0.74392	0.74382	0.74385	0.74373	0.74361	0.74348	
00.30	C.73086	0.73079	0.73071	0.73047	0.73037	0.73040	0.73029	0.73016	0.73003	
00.34	C.70526	0.70519	0.70510	0.70485	0.70474	0.70479	0.70467	0.70453	0.70439	
00.38	C.68122	0.68115	0.68107	0.68079	0.68068	0.68075	0.68063	0.68049	0.68034	
00.42	C.65862	0.65856	0.65848	0.65819	0.65808	0.65817	0.65805	0.65791	0.65776	
00.46	C.63735	0.63730	0.63723	0.63691	0.63681	0.63692	0.63679	0.63665	0.63650	
00.50	C.61728	0.61723	0.61717	0.61683	0.61672	0.61686	0.61672	0.61657	0.61641	
00.54	C.59829	0.59824	0.59817	0.59781	0.59770	0.59785	0.59771	0.59755	0.59738	
00.58	C.58026	0.58021	0.58014	0.57975	0.57963	0.57980	0.57965	0.57948	0.57929	
00.62	C.56310	0.56305	0.56298	0.56256	0.56244	0.56261	0.56245	0.56227	0.56208	
00.66	C.54674	0.54669	0.54661	0.54617	0.54604	0.54623	0.54606	0.54587	0.54566	
00.70	C.53113	0.53107	0.53099	0.53052	0.53038	0.53058	0.53040	0.53020	0.52998	
00.78	C.50190	0.50184	0.50175	0.50122	0.50107	0.50130	0.50111	0.50089	0.50065	
00.86	C.47505	0.47499	0.47489	0.47432	0.47416	0.47443	0.47422	0.47399	0.47374	
00.94	C.45032	0.45026	0.45017	0.44956	0.44940	0.44971	0.44951	0.44928	0.44903	
01.02	C.42751	0.42747	0.42735	0.42676	0.42662	0.42698	0.42678	0.42656	0.42632	
01.10	C.40648	0.40647	0.40642	0.40577	0.40564	0.40605	0.40587	0.40566	0.40543	
01.18	C.38707	0.38708	0.38705	0.38639	0.38628	0.38674	0.38658	0.38637	0.38615	
01.26	C.36910	0.36914	0.36913	0.36844	0.36834	0.36886	0.36870	0.36851	0.36829	
01.34	C.35241	0.35247	0.35248	0.35177	0.35169	0.35225	0.35210	0.35192	0.35170	
01.42	C.33687	0.33695	0.33698	0.33626	0.33619	0.33680	0.33666	0.33648	0.33627	
01.50	C.32238	0.32249	0.32254	0.32180	0.32174	0.32241	0.32228	0.32211	0.32190	
01.66	C.29626	0.29642	0.29652	0.29574	0.29572	0.29649	0.29637	0.29621	0.29600	
01.82	C.27348	0.27369	0.27383	0.27300	0.27299	0.27383	0.27371	0.27352	0.27328	
01.98	C.25352	0.25375	0.25390	0.25299	0.25296	0.25385	0.25369	0.25346	0.25316	
02.14	C.23589	0.23612	0.23625	0.23523	0.23516	0.23608	0.23586	0.23556	0.23519	
02.30	C.22020	0.22040	0.22049	0.21936	0.21923	0.22017	0.21988	0.21951	0.21908	
02.46	C.20616	0.20633	0.20638	0.20511	0.20493	0.20590	0.20555	0.20512	0.20462	
02.62	C.19358	0.19371	0.19372	0.19232	0.19209	0.19308	0.19267	0.19217	0.19160	
02.78	C.18228	0.18237	0.18233	0.18080	0.18050	0.18150	0.18102	0.18045	0.17979	
02.94	C.17209	0.17213	0.17203	0.17035	0.16998	0.17098	0.17041	0.16973	0.16898	
03.10	C.16284	0.16281	0.16263	0.16079	0.16033	0.16131	0.16064	0.15987	0.15901	
03.42	C.14658	0.14638	0.14601	0.14384	0.14318	0.14410	0.14324	0.14228	0.14124	
03.74	C.13261	0.13223	0.13167	0.12920	0.12837	0.12925	0.12823	0.12712	0.12595	
04.06	C.12047	0.11992	0.11921	0.11649	0.11553	0.11639	0.11526	0.11407	0.11282	
04.38	C.10985	0.10917	0.10834	0.10544	0.10439	0.10525	0.10406	0.10282	0.10154	
04.70	C.10053	0.09975	0.09884	0.09582	0.09472	0.09558	0.09437	0.09311	0.09183	
05.02	C.09233	0.09148	0.09052	0.08744	0.08632	0.08718	0.08597	0.08473	0.08347	
05.34	C.08510	0.08421	0.08321	0.08012	0.07900	0.07987	0.07868	0.07746	0.07624	
05.66	C.07872	0.07781	0.07681	0.07373	0.07262	0.07350	0.07234	0.07116	0.06998	
05.98	C.07309	0.07217	0.07118	0.06814	0.06705	0.06793	0.06680	0.06567	0.06454	
06.30	C.06813	0.06721	0.06623	0.06323	0.06218	0.06305	0.06196	0.06087	0.05978	
06.94	C.05984	0.05893	0.05797	0.05509	0.05409	0.05493	0.05391	0.05290	0.05190	
07.58	C.05321	0.05231	0.05136	0.04864	0.04769	0.04846	0.04750	0.04656	0.04564	
08.22	C.04776	0.04685	0.04593	0.04339	0.04249	0.04316	0.04227	0.04140	0.04056	
08.86	C.04316	0.04226	0.04137	0.03903	0.03818	0.03875	0.03792	0.03712	0.03635	
09.50	C.03921	0.03834	0.03748	0.03534	0.03455	0.03502	0.03425	0.03351	0.03280	
10.14	C.03578	0.03494	0.03412	0.03219	0.03144	0.03182	0.03111	0.03043	0.02978	
10.78	C.03278	0.03198	0.03120	0.02945	0.02875	0.02905	0.02840	0.02777	0.02718	
11.42	C.03014	0.02937	0.02865	0.02706	0.02641	0.02664	0.02604	0.02546	0.02492	
12.06	C.02780	0.02708	0.02640	0.02495	0.02434	0.02454	0.02398	0.02346	0.02296	

U(X) X	PA 91	U 92	NP 93	PU 94	AM 95	CM 96	BK 97	CF 98	E 99
12.70	0.02574	0.02506	0.02442	0.02308	0.02252	0.02270	0.02219	0.02170	0.02125
13.98	0.02230	0.02171	0.02116	0.01999	0.01951	0.01969	0.01927	0.01886	0.01848
15.26	0.01964	0.01913	0.01867	0.01762	0.01721	0.01743	0.01708	0.01674	0.01643
16.54	0.01761	0.01718	0.01678	0.01584	0.01550	0.01574	0.01544	0.01516	0.01489
17.82	0.01605	0.01568	0.01534	0.01454	0.01425	0.01445	0.01419	0.01395	0.01372
19.10	0.01483	0.01450	0.01421	0.01355	0.01330	0.01342	0.01320	0.01298	0.01278
20.38	0.01384	0.01354	0.01328	0.01277	0.01255	0.01257	0.01237	0.01217	0.01198
21.66	0.01299	0.01272	0.01248	0.01211	0.01191	0.01183	0.01164	0.01146	0.01129
22.94	0.01225	0.01200	0.01178	0.01153	0.01134	0.01118	0.01100	0.01083	0.01067
24.22	0.01155	0.01136	0.01115	0.01101	0.01083	0.01058	0.01042	0.01026	0.01010
25.50	0.01099	0.01087	0.01075	0.01064	0.01053	0.01042	0.01031	0.01020	0.01010
28.06	0.01099	0.01087	0.01075	0.01064	0.01053	0.01042	0.01031	0.01020	0.01010
30.62	0.01099	0.01087	0.01075	0.01064	0.01053	0.01042	0.01031	0.01020	0.01010
33.18	0.01099	0.01087	0.01075	0.01064	0.01053	0.01042	0.01031	0.01020	0.01010
35.74	0.01099	0.01087	0.01075	0.01064	0.01053	0.01042	0.01031	0.01020	0.01010
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(-E)	7242.8	7409.2	2577.5	7747.2	7919.2	8093.6	8269.4	8447.2	8626.8
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(-E)	1218.1	1249.5	1281.3	1313.1	1345.6	1379.1	1412.4	1446.2	1480.4
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(-E)	317.28	326.64	336.10	345.20	354.89	365.21	375.21	385.21	395.39
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(-E)	297.53	306.58	315.73	324.52	333.89	343.89	353.52	363.26	373.12
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(-E)	260.35	268.81	277.37	285.56	294.34	303.75	312.77	321.92	331.18
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(-E)	80.22	83.16	86.12	88.63	91.63	95.16	98.23	101.33	104.46
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(-E)	71.064	73.819	76.594	78.918	81.734	85.078	87.960	90.873	93.815
SHELL (4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(-E)	53.910	56.308	58.725	60.689	63.143	66.126	68.644	71.192	73.768
SHELL (4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14
(-E)	30.088	31.954	33.838	35.265	37.184	39.633	41.613	43.622	45.657
SHELL (5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(-E)	17.767	18.490	19.205	19.467	20.157	21.308	22.002	22.695	23.385
SHELL (5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6
(-E)	14.224	14.844	15.456	15.623	16.209	17.251	17.842	18.432	19.019
SHELL (5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10
(-E)	8.019	8.438	8.850	8.838	9.226	10.050	10.443	10.834	11.222
SHELL (5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2	(5F) 2
(-E)	1.0672	1.1830	1.2952	1.0727	1.1654	1.6156	1.7179	1.8190	1.9181
SHELL (6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2
(-E)	2.8808	2.9631	3.0399	2.9033	2.9680	3.2515	3.3164	3.3795	3.4409
SHELL (6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6
(-E)	1.8678	1.9181	1.9639	1.8311	1.8674	2.0876	2.1241	2.1595	2.1934
SHELL (6D) 1	(6D) 1	(6D) 1	(6D) 1	(6D) 0	(6D) 0	(6D) 1	(6D) 1	(6D) 1	(6D) 1
(-E)	0.4449	0.4494	0.4516	0.	0.	0.4540	0.4526	0.4512	0.4490
SHELL (7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2
(-E)	0.3492	0.3530	0.3564	0.3357	0.3387	0.3661	0.3690	0.3720	0.3749
U(X) X	NI 28	CE 58	TB 65	BK 97	CF 98	E 99	FM100	MV101	NO102
00.00	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
00.01	0.99006	0.98893	0.98872	0.98813	0.98811	0.98810	0.98808	0.98807	0.98805
00.02	0.97988	0.97766	0.97725	0.97613	0.97610	0.97607	0.97604	0.97602	0.97599
00.03	0.96959	0.96640	0.96582	0.96427	0.96424	0.96420	0.96416	0.96412	0.96408
00.04	0.95928	0.95527	0.95455	0.95267	0.95263	0.95258	0.95253	0.95248	0.95244
00.05	0.94903	0.94435	0.94350	0.94136	0.94131	0.94126	0.94120	0.94115	0.94109
00.06	0.93887	0.93365	0.93270	0.93035	0.93029	0.93023	0.93017	0.93011	0.93005
00.07	0.92885	0.92319	0.92215	0.91962	0.91955	0.91949	0.91943	0.91936	0.91929

U(X)	X	NI 28	CE 58	TB 65	BK 97	CF 98	E 99	FM100	MV101	NO1022
00.08	0.91895	0.91297	0.91184	0.90917	0.90910	0.90904	0.90897	0.90890	0.90883	
00.09	0.90928	0.90298	0.90177	0.89899	0.89893	0.89886	0.89878	0.89871	0.89864	
00.10	0.89975	0.89321	0.89194	0.88909	0.88902	0.88895	0.88888	0.88880	0.88872	
00.12	0.88120	0.87434	0.87296	0.87006	0.86999	0.86992	0.86984	0.86976	0.86968	
00.14	0.86331	0.85632	0.85487	0.85197	0.85190	0.85182	0.85174	0.85166	0.85157	
00.16	0.84606	0.83913	0.83763	0.83470	0.83462	0.83453	0.83444	0.83435	0.83426	
00.18	0.82942	0.82272	0.82116	0.81811	0.81802	0.81793	0.81784	0.81774	0.81763	
00.20	0.81336	0.80701	0.80538	0.80215	0.80205	0.80195	0.80185	0.80174	0.80162	
00.22	0.79787	0.79193	0.79020	0.78675	0.78664	0.78653	0.78642	0.78630	0.78618	
00.24	0.78294	0.77741	0.77555	0.77187	0.77176	0.77165	0.77153	0.77140	0.77127	
00.26	0.76856	0.76338	0.76140	0.75750	0.75738	0.75726	0.75713	0.75700	0.75686	
00.28	0.75472	0.74982	0.74770	0.74359	0.74347	0.74334	0.74321	0.74307	0.74292	
00.30	0.74138	0.73668	0.73442	0.73014	0.73001	0.72988	0.72973	0.72959	0.72943	
00.34	0.71611	0.71159	0.70908	0.70449	0.70436	0.70422	0.70407	0.70391	0.70374	
00.38	0.69246	0.68797	0.68520	0.68043	0.68029	0.68015	0.67999	0.67982	0.67965	
00.42	0.67020	0.66567	0.66266	0.65783	0.65769	0.65754	0.65738	0.65721	0.65703	
00.46	0.64913	0.64458	0.64137	0.63655	0.63641	0.63625	0.63608	0.63590	0.63571	
00.50	0.62912	0.62464	0.62124	0.61646	0.61631	0.61615	0.61597	0.61578	0.61557	
00.54	0.61005	0.60576	0.60222	0.59743	0.59727	0.59709	0.59690	0.59670	0.59648	
00.58	0.59194	0.58790	0.58422	0.57934	0.57917	0.57898	0.57878	0.57854	0.57833	
00.62	0.57463	0.57100	0.56718	0.56213	0.56194	0.56174	0.56153	0.56130	0.56105	
00.66	0.55809	0.55498	0.55100	0.54571	0.54551	0.54530	0.54508	0.54483	0.54457	
00.70	0.54226	0.53979	0.53561	0.53003	0.52983	0.52960	0.52936	0.52910	0.52883	
00.78	0.51252	0.51160	0.50694	0.50069	0.50047	0.50023	0.49996	0.49968	0.49939	
00.86	0.48505	0.48595	0.48072	0.47376	0.47353	0.47327	0.47300	0.47271	0.47240	
00.94	0.45953	0.46248	0.45662	0.44901	0.44877	0.44852	0.44824	0.44795	0.44764	
01.02	0.43578	0.44093	0.43439	0.42624	0.42602	0.42577	0.42550	0.42521	0.42490	
01.10	0.41366	0.42106	0.41377	0.40529	0.40508	0.40484	0.40458	0.40429	0.40398	
01.18	0.39310	0.40267	0.39457	0.38596	0.38575	0.38552	0.38526	0.38497	0.38466	
01.26	0.37400	0.38556	0.37663	0.36804	0.36784	0.36761	0.36736	0.36707	0.36676	
01.34	0.35624	0.36959	0.35982	0.35141	0.35121	0.35099	0.35073	0.35045	0.35013	
01.42	0.33968	0.35460	0.34407	0.33593	0.33574	0.33552	0.33526	0.33498	0.33466	
01.50	0.32416	0.34053	0.32933	0.32151	0.32133	0.32111	0.32086	0.32057	0.32025	
01.66	0.29576	0.31492	0.30261	0.29552	0.29535	0.29513	0.29486	0.29456	0.29421	
01.82	0.27028	0.29240	0.27902	0.27278	0.27258	0.27233	0.27203	0.27168	0.27127	
01.98	0.24731	0.27254	0.25792	0.25268	0.25244	0.25213	0.25176	0.25134	0.25085	
02.14	0.22662	0.25480	0.23888	0.23477	0.23446	0.23408	0.23363	0.23312	0.23255	
02.30	0.20803	0.23872	0.22164	0.21871	0.21833	0.21788	0.21736	0.21678	0.21614	
02.46	0.19138	0.22401	0.20604	0.20430	0.20385	0.20334	0.20275	0.20209	0.20138	
02.62	0.17649	0.21051	0.19196	0.19133	0.19082	0.19023	0.18957	0.18883	0.18803	
02.78	0.16321	0.19812	0.17925	0.17960	0.17901	0.17834	0.17759	0.17676	0.17585	
02.94	0.15135	0.18676	0.16777	0.16890	0.16822	0.16745	0.16660	0.16566	0.16466	
03.10	0.14076	0.17632	0.15735	0.15907	0.15828	0.15741	0.15645	0.15542	0.15432	
03.42	0.12281	0.15794	0.13945	0.14152	0.14055	0.13950	0.13837	0.13717	0.13592	
03.74	0.10832	0.14233	0.12457	0.12639	0.12528	0.12410	0.12285	0.12155	0.12021	
04.06	0.09651	0.12901	0.11216	0.11334	0.11214	0.11088	0.10957	0.10823	0.10686	
04.38	0.08677	0.11763	0.10175	0.10207	0.10082	0.09954	0.09822	0.09687	0.09550	
04.70	0.07866	0.10791	0.09297	0.09234	0.09109	0.08980	0.08849	0.08717	0.08584	
05.02	0.07185	0.09960	0.08548	0.08393	0.08269	0.08143	0.08015	0.07887	0.07760	
05.34	0.06607	0.09245	0.07900	0.07665	0.07543	0.07421	0.07298	0.07176	0.07054	
05.66	0.06115	0.08621	0.07334	0.07032	0.06915	0.06797	0.06680	0.06563	0.06447	
05.98	0.05692	0.08069	0.06833	0.06482	0.06369	0.06256	0.06144	0.06033	0.05923	
06.30	0.05327	0.07575	0.06386	0.06002	0.05893	0.05785	0.05678	0.05573	0.05469	
06.94	0.04731	0.06721	0.05621	0.05207	0.05107	0.05008	0.04911	0.04816	0.04723	
07.58	0.04269	0.06005	0.04992	0.04580	0.04488	0.04397	0.04309	0.04223	0.04140	
08.22	0.03902	0.05395	0.04466	0.04073	0.03988	0.03905	0.03825	0.03747	0.03672	
08.86	0.03606	0.04872	0.04022	0.03654	0.03576	0.03501	0.03427	0.03357	0.03289	
09.50	0.03571	0.04420	0.03644	0.03303	0.03231	0.03162	0.03095	0.03031	0.02970	

U(X) X	NI 28	CE 58	TR 65	BK 97	CF 98	E 99	FM100	MV101	ND102
10.14	0.03571	0.04029	0.03322	0.03003	0.02937	0.02874	0.02813	0.02754	0.02698
10.78	0.03571	0.03691	0.03048	0.02745	0.02694	0.02626	0.02570	0.02516	0.02465
11.42	0.03571	0.03401	0.02817	0.02520	0.02463	0.02410	0.02358	0.02309	0.02263
12.06	0.03571	0.03152	0.02622	0.02322	0.02270	0.02221	0.02174	0.02129	0.02086
12.70	0.03571	0.02940	0.02459	0.02148	0.02100	0.02055	0.02012	0.01971	0.01932
13.98	0.03571	0.02608	0.02204	0.01863	0.01822	0.01784	0.01748	0.01714	0.01681
15.26	0.03571	0.02363	0.02013	0.01647	0.01613	0.01582	0.01552	0.01523	0.01497
16.54	0.03571	0.02174	0.01861	0.01489	0.01461	0.01434	0.01410	0.01386	0.01364
17.82	0.03571	0.02020	0.01733	0.01373	0.01349	0.01327	0.01306	0.01285	0.01266
19.10	0.03571	0.01887	0.01620	0.01285	0.01264	0.01245	0.01226	0.01208	0.01191
20.38	0.03571	0.01769	0.01538	0.01214	0.01195	0.01178	0.01161	0.01144	0.01129
21.66	0.03571	0.01724	0.01538	0.01154	0.01136	0.01120	0.01104	0.01089	0.01074
22.94	0.03571	0.01724	0.01538	0.01100	0.01083	0.01068	0.01053	0.01038	0.01024
24.22	0.03571	0.01724	0.01538	0.01050	0.01034	0.01020	0.01005	0.00992	0.00980
25.50	0.03571	0.01724	0.01538	0.01031	0.01020	0.01010	0.01000	0.00990	0.00980
28.06	0.03571	0.01724	0.01538	0.01031	0.01020	0.01010	0.01000	0.00990	0.00980
30.62	0.03571	0.01724	0.01538	0.01031	0.01020	0.01010	0.01000	0.00990	0.00980
33.18	0.03571	0.01724	0.01538	0.01031	0.01020	0.01010	0.01000	0.00990	0.00980
35.74	0.03571	0.01724	0.01538	0.01031	0.01020	0.01010	0.01000	0.00990	0.00980
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2	(1S) 2
(-E) 603.2	2830.8	3591.9	8268.9	8446.7	8626.4	8807.9	8991.3	9176.6	
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2	(2S) 2
(-E) 72.0	443.3	577.4	1455.0	1489.3	1523.9	1559.0	1594.4	1630.3	
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6	(2P) 6
(-E) 63.3	420.3	550.9	1411.9	1445.7	1479.8	1514.4	1549.3	1584.6	
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2	(3S) 2
(-E) 8.02	96.43	128.79	374.62	384.67	394.83	405.12	415.53	426.06	
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6	(3P) 6
(-E) 5.29	86.32	116.77	352.99	362.72	372.57	382.53	392.62	402.84	
SHELL (3D) 9	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10	(3D) 10
(-E) 0.69	67.32	94.18	312.25	321.38	330.62	339.99	349.48	359.08	
SHELL (4S) 1	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2	(4S) 2
(-E) 0.49	19.82	25.82	97.72	100.80	103.92	107.07	110.25	113.46	
SHELL (4P) 0	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6	(4P) 6
(-E) 0.	16.00	21.03	87.44	90.34	93.27	96.23	99.22	102.24	
SHELL (4D) 0	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10	(4D) 10
(-E) 0.	9.215	12.384	68.127	70.661	73.223	75.815	78.437	81.089	
SHELL (4F) 0	(4F) 1	(4F) 8	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14	(4F) 14
(-E) 0.	1.236	1.630	41.093	43.087	45.108	47.157	49.234	51.340	
SHELL (5S) 0	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2	(5S) 2
(-E) 0.	3.067	3.647	21.523	22.202	22.879	23.555	24.231	24.906	
SHELL (5P) 0	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6	(5P) 6
(-E) 0.	1.990	2.311	17.370	17.946	18.520	19.093	19.665	20.237	
SHELL (5D) 0	(5D) 1	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10	(5D) 10
(-E) 0.	0.455	0.430	9.589	10.367	10.742	11.116	11.489	11.860	
SHELL (5F) 0	(5F) 0	(5F) 0	(5F) 9	(5F) 10	(5F) 11	(5F) 12	(5F) 13	(5F) 14	(5F) 14
(-E) 0.	0.	0.	1.3438	1.4304	1.5154	1.5990	1.6808	1.7616	
SHELL (6S) 0	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2	(6S) 2
(-E) 0.	0.3623	0.3918	3.0885	3.1454	3.2006	3.2541	3.3062	3.3570	
SHELL (6P) 0	(6P) 0	(6P) 0	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6	(6P) 6
(-E) 0.	0.	0.	1.9327	1.9628	1.9914	2.0188	2.0449	2.0700	
SHELL (7S) 0	(7S) 0	(7S) 0	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2	(7S) 2
(-E) 0.	0.	0.	0.3438	0.3462	0.3486	0.3509	0.3531	0.3552	
U(X) X	FM100	MV101	ND102	LW103					
00.00	1.00000	1.00000	1.00000	1.00000					
00.01	0.98809	0.98807	0.98806	0.98804					
00.02	0.97605	0.97603	0.97600	0.97597					
00.03	0.96417	0.96413	0.96409	0.96405					

U(X)	X	FM100	MV101	NO102	LW103
00.04	C.95255	0.95250	0.95245	C.95241	
00.05	C.94123	0.94117	0.94112	C.94106	
00.06	C.93020	0.93014	0.93008	C.93001	
00.07	C.91946	0.91939	0.91933	C.91926	
00.08	C.90901	0.90894	0.90887	0.90879	
00.09	C.89883	0.89876	0.89868	C.89861	
00.10	C.88892	0.88885	0.88877	C.88870	
00.12	C.86990	0.86982	0.86974	C.86966	
00.14	C.85181	0.85173	0.85164	C.85156	
00.16	C.83452	0.83443	0.83434	C.83425	
00.18	C.81793	0.81783	0.81773	C.81762	
00.20	C.80195	0.80184	0.80173	C.80161	
00.22	C.78653	0.78642	0.78630	C.78617	
00.24	C.77165	0.77152	0.77139	C.77126	
00.26	C.75726	0.75713	0.75699	C.75685	
00.28	C.74335	0.74321	0.74307	C.74291	
00.30	C.72989	0.72974	0.72959	C.72943	
00.34	C.70424	0.70409	0.70392	C.70375	
00.38	C.68019	0.68003	0.67986	C.67968	
00.42	C.65760	0.65743	0.65725	C.65707	
00.46	C.63633	0.63615	0.63597	C.63577	
00.50	C.61624	0.61605	0.61585	C.61564	
00.54	C.59719	0.59699	0.59678	C.59655	
00.58	C.57909	0.57888	0.57865	C.57841	
00.62	C.56187	0.56164	0.56139	C.56114	
00.66	C.54544	0.54519	0.54494	C.54466	
00.70	C.52975	0.52949	0.52922	C.52893	
00.78	C.50039	0.50011	0.49982	C.49951	
00.86	C.47347	0.47318	0.47288	C.47255	
00.94	C.44876	0.44847	0.44816	C.44783	
01.02	C.42606	0.42577	0.42547	C.42514	
01.10	C.40517	0.40489	0.40459	C.40427	
01.18	C.38589	0.38562	0.38531	C.38499	
01.26	C.36804	0.36776	0.36745	C.36712	
01.34	C.35145	0.35117	0.35087	C.35053	
01.42	C.33602	0.33575	0.33544	C.33510	
01.50	C.32166	0.32138	0.32106	C.32072	
01.66	C.29574	0.29544	0.29510	C.29472	
01.82	C.27299	0.27265	0.27225	C.27180	
01.98	C.25280	0.25239	0.25191	C.25138	
02.14	C.23476	0.23426	0.23370	C.23309	
02.30	C.21857	0.21800	0.21737	C.21668	
02.46	C.20404	0.20340	0.20270	C.20194	
02.62	C.19095	0.19023	0.18944	C.18859	
02.78	C.17905	0.17823	0.17735	C.17639	
02.94	C.16814	0.16722	0.16623	C.16517	
03.10	C.15807	0.15705	0.15597	C.15482	
03.42	C.14012	0.13894	0.13770	C.13641	
03.74	C.12472	0.12344	0.12211	C.12074	
04.06	C.11153	0.11019	0.10883	C.10745	
04.38	C.10023	0.09889	0.09753	C.09616	
04.70	C.09053	0.08922	0.08785	C.08656	
05.02	C.08220	0.08092	0.07965	C.07838	
05.34	C.07501	0.07379	0.07257	C.07136	
05.66	C.06880	0.06763	0.06648	C.06533	
05.98	C.06341	0.06230	0.06120	C.06012	
06.30	C.05870	0.05764	0.05660	C.05558	
06.94	C.05092	0.04995	0.04901	C.04810	

U(X) X	FM100	MV101	NO102	LW103
07.58	0.04475	0.04387	0.04303	0.04220
08.22	0.03974	0.03895	0.03815	0.03745
08.86	0.03560	0.03488	0.03419	0.03353
09.50	0.03212	0.03147	0.03084	0.03024
10.14	0.02916	0.02856	0.02799	0.02745
10.78	0.02661	0.02607	0.02555	0.02505
11.42	0.02440	0.02390	0.02343	0.02298
12.06	0.02248	0.02203	0.02160	0.02119
12.70	0.02081	0.02040	0.02001	0.01964
13.98	0.01813	0.01779	0.01746	0.01716
15.26	0.01613	0.01585	0.01558	0.01533
16.54	0.01464	0.01440	0.01418	0.01397
17.82	0.01350	0.01329	0.01310	0.01291
19.10	0.01258	0.01240	0.01222	0.01205
20.38	0.01181	0.01164	0.01148	0.01132
21.66	0.01113	0.01097	0.01082	0.01067
22.94	0.01051	0.01037	0.01022	0.01009
24.22	0.01000	0.00990	0.00980	0.00971
SHELL (1S) 2	(1S) 2	(1S) 2	(1S) 2	
(=E) 8808.4	8991.8	9177.1	9364.3	
SHELL (2S) 2	(2S) 2	(2S) 2	(2S) 2	
(=E) 1559.5	15.950	1630.9	1667.1	
SHELL (2P) 6	(2P) 6	(2P) 6	(2P) 6	
(=E) 1514.9	1549.8	1585.2	1620.9	
SHELL (3S) 2	(3S) 2	(3S) 2	(3S) 2	
(=E) 405.69	416.11	426.66	437.33	
SHELL (3P) 6	(3P) 6	(3P) 6	(3P) 6	
(=E) 383.10	393.21	403.43	413.78	
SHELL (3D) 10	(3D) 10	(3D) 10	(3D) 10	
(=E) 340.56	350.06	359.68	369.41	
SHELL (4S) 2	(4S) 2	(4S) 2	(4S) 2	
(=E) 107.63	110.82	114.05	117.31	
SHELL (4P) 6	(4P) 6	(4P) 6	(4P) 6	
(=E) 96.79	99.79	102.83	105.90	
SHELL (4D) 10	(4D) 10	(4D) 10	(4D) 10	
(=E) 76.374	79.010	81.676	84.373	
SHELL (4F) 14	(4F) 14	(4F) 14	(4F) 14	
(=E) 47.720	49.811	51.931	54.080	
SHELL (5S) 2	(5S) 2	(5S) 2	(5S) 2	
(=E) 24.074	24.763	25.452	26.141	
SHELL (5P) 6	(5P) 6	(5P) 6	(5P) 6	
(=E) 19.605	20.190	20.775	21.360	
SHELL (5D) 10	(5D) 10	(5D) 10	(5D) 10	
(=E) 11.609	11.995	12.380	12.765	
SHELL (5F) 11	(5F) 12	(5F) 13	(5F) 14	
(=E) 2.0159	2.1122	2.2073	2.3011	
SHELL (6S) 2	(6S) 2	(6S) 2	(6S) 2	
(=E) 3.5008	3.5593	3.6167	3.6731	
SHELL (6P) 6	(6P) 6	(6P) 6	(6P) 6	
(=E) 2.2262	2.2578	2.2885	2.3183	
SHELL (6D) 1	(6D) 1	(6D) 1	(6D) 1	
(=E) 0.4463	0.4432	0.4397	0.4358	
SHELL (7S) 2	(7S) 2	(7S) 2	(7S) 2	
(=E) 0.3777	0.3805	0.3832	0.3859	